# WASP AT - Wasp Analysis Tools

# WASP Inputs Description

**Developed by:**

**Integrated Decision Support Group**
**The Water Center**
**Colorado State University**
**Fort Collins, Colorado**

**Developed for:**

**U.S Department of the Interior**
**Bureau of Reclamation**
**Technical Services Center**
**Denver, Colorado**

# 1.0 Table of Contents

# 2.0 Introduction to Inputs Description

This document has been assembled from the WASP5 user documentation to summarize the input requirement for the model and as a tool for development efforts for WASP Analysis Tools. For more information on the WASP5 program:

WASP5 is used by federal government personnel and private users to model water quality parameters in streams. Current methods for preparing input files are cumbersome and often become the major task of a water quality modeling projects. This Graphical Data Processor (GDP) has been designed to receive standard inputs from WATSTORE, STORET, and supplemental data in the form of delimited ASCII files. These data inputs can be pasted into Wasp Builder to created input files for WASP5.

WASP has been used to simulate the water quality and pollutant fate for a variety of aquatic systems. It is used primarily to investigate the water quality response to management actions, primarily point and non-point source load reduction. It is presently being distributed by EPA-Office of Research and Development/ Center for Exposure Assessment Modeling Athens, GA (CEAM).

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# 3.0 DYNHYD5 Inputs by Card

## 3.1 Data Group A: Simulation Control

Each record in Data Group A is input once; therefore, Data Group A consists of 4 lines of data. Data Group B starts on the 5th line (no blank line).

**Table 1: DATA GROUP A: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Title of Simulation (A80)**<br>ALPHA(1), ALPHA(2), and HEADER assist the user in maintaining a log of computer simulations, but are not actually used by the DYNHYD5 program.<br>P | |
| ALPHA(J) | alphanumeric characters to identify the system, date and run number. (20A4) | P |
| **Record 2** | **Description of Simulation (A80)** | |
| ALPHA(J) | alphanumeric characters to identify the system, date and run number. (20A4) | P |
| **Record 3** | **Data Group Identification (A80)** | |
| HEADER | alphanumeric characters to identify the data group, “PROGRAM CONTROL DATA.” (20A4) | P |
| **Record 4** | **Simulation Control Data (3I5, F5.0, I5, F5.0, F3.0 F2.0, F5.0, F3.0 F2.0)** | |
| NJ | number of junctions in the model network. (I5) | N |
| NC | number of channels in the model network. (I5) | N |
| NCYC | total number of time steps for execution (number of cycles). If equal to zero, the model will compute NCYC internally (cycles). (I5) | T |
| DELT | time interval used in execution (sec). Note that it is important that the time step meet the Courant condition, that is, it should be less than the shortest channel length divided by the wave celerity (see equation 29 in section 1.5.2 above). (F5.0) | T |

**Table 1: DATA GROUP A: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| ICRD | file containing the initial conditions for junctions and channels. If equal to 0 or 5, data set is read. If equal to 8, a file 8, previously created by subroutine RESTART, is read. (I5) | N |
| ZDAY | beginning day of simulation (day). (F5.0) | T |
| ZHR | beginning hour of simulation (hr). (F3.0) | T |
| ZMIN | beginning minute of simulation (min). (F2.0) | T |
| EDAY | ending day of simulation (day). (F5.0) | T |
| EHR | ending hour of simulation (hr). (F3.0) | T |
| EMIN | ending minute of simulation (min). (F2.0) | T |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.2 Data Group B: Printout Control

**Table 2: DATA GROUP B: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (20A4) - (Records 1 and 2 are entered once)** | |
| HEADER | alphanumeric characters to identify the data group, “PRINTOUT CONTROL DATA.” (20A4) | enter: “Printout Control Data.” |
| **Record 2** | **Output Control Information (2F10.0, I5)** | |
| FPRINT | time for printout to begin (hr). (F10.0) | T |
| PINTVL | time interval between printouts (hr). (F10.0) | T |
| NOPRT | number of junctions for which printouts (results) are desired, can be 1 through NJ. (I5) | P |
| **Record 3** | **List of Junctions (15I5) - (Record 3 may contain several lines depending upon NOPRT. One line may contain up to 16 entries. Therefore, if NOPRT is equal to 1-16, then Record 3 will consist of 1 line. If NOPRT is equal to 17-32, then Record 3 will consist of 2 lines, etc. The total number of lines for Data Group B equals 2 + (1 + INT((NOPRT-1)/ 16)))** | |
| JPRT(I) | junction number for results to be printed. (I5) | N |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.3 Data Group C: Hydraulic Summary

**Table 3: Data Group C: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (20A4)** | |
| HEADER | alphanumeric characters to identify the data group "Summary Control Data." (A4) | enter: "Summary Control Data." |
| **Record 2** | **Summary Control Data (I5, F5.0, F3.0, F2.0, 2F5.0)** | |
| SUMRY | option number that controls how the hydrodynamic scratch file (file 2) is processed to create a permanent summary file (file 4) for the water quality model to read. If equal to zero, then no summary file will be created. If equal to 1, a formatted file will be created. (I5) | SUMRY =1 |
| TDAY | day to begin storing parameters to file (day). (5.0) | T |
| THR | hour to begin storing parameters to file (hr). (F3.0) | T |
| TMIN | minute to begin storing parameters to file (min). (F2.0) | T |
| DTDUMP | time interval for storing intermediate results in scratch file; usually 12.5, 24.0, or 25.0 hours (hr). (F5.0) | T |
| NODYN | number of hydraulic time steps per quality time steps desired. (F5.0) | T |
| INTSCR | frequency with which to store hydraulic data on scratch file, measured in hydraulic time steps. (f5.0) | T |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.4 Data Group D: Junction Data

**Table 4: DATA GROUP D: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (20A4) - (entered once)** | |
| HEADER | alphanumeric characters to identify the data group, "JUNCTION DATA." (20A4) | enter: "Junction Data." |
| **Record 2** | **Junction Data (I5, 3F10.0, 6I5) - (entered NJ times (NJ = number of junctions))** | |
| JJ | junction number. (I5) | N |
| Y(J) | initial head (or surface elevation) in reference to a horizontal model datum, at junction JJ (m). (F10.0) | N |
| SURF(J) | surface area at junction JJ ($m^2$). (F10.0) | N |
| BELEV(J) | bottom elevation above (or below) the horizontal datum plane (usually taken to be mean sea level) (m). (F10.0) | N |
| NCHAN(J,I) | channel number entering junction JJ. Maximum number of channels entering any one junction is six (I = 1 - 6). Start list with lowest channel number. (I5) | N |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.5 Data Group E: Channel Data

A channel may only connect two junctions. Therefore, only NJUNC(N,1) and NJUNC(N,2) exists.

**Table 5: DATA GROUP E: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (20A4) - (entered only once)** | |
| HEADER | alphanumeric characters to identify the data group, "CHANNEL DATA." (20A4) | enter: "Channel Data." |
| **Record 2** | **Channel Data (I5, 6F10.0, 2I5)** | |
| NN | channel number. (I5) | S |
| CLEN(N) | length of channel NN (m). (F10.0) | S |
| B(N) | width of channel NN (m). (F10.0) | S |

**Table 5: DATA GROUP E: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| R(N) | hydraulic radius or depth of channel NN (m). (F10.0) | S |
| CDIR(N) | channel direction, or angle in degrees measured from true north. The channel direction points in the direction of positive flow, from the higher junction number to the lower junction number (degrees).(F10.0) | S |
| CN(N) | Manning roughness coefficient for channel NN (sec. $m^{-1/3}$). Ranges from 0.01 to 0.08. (F10.0) | S |
| V(N) | the initial mean velocity in channel NN, m/sec. (F10.0) | S |
| NJUNC(N,1) | the connecting junction at the lower end of channel NN. (I5) | S, N |
| NJUNC(N,2) | the connecting junction at the higher end of channel NN. (I5) | S, N |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.6 Data Group F: Inflow Data

Records 1 and 2 are entered once in Data Group F. Record 3 is entered NCFLOW times with one junction number and one flow per line. Records 4 and 5 are entered once in Data Group F. Record 6 is entered NVFLOW times, but not consecutively. Record 6 should be entered (one junction, one number of breaks), then Record 7 with 4 flows per line until NINCR(I) flows have been entered. Then Record 6 entered again followed by Record 7.

**Table 6: DATA GROUP F: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (20A4)** | |
| HEADER | alphanumeric characters to identify the data group and type of inflows, "CONSTANT INFLOW DATA." (20A4) | enter: "Constant Inflow Data." |
| **Record 2** | **Constant Inflow Number (I5)** | |
| NCFLOW | the number of constant inflows that will be read. (I5)<br>If NCFLOW = 0, skip to Record 4. | N |
| **Record 3** | **Constant Inflow Data (I10, F10.0)** | |
| JRCF(I) | junction that will be receiving the following inflow. (I10) | N |
| CFLOW(I) | the value of the constant inflow into junction JRCF(I) ($m^3$/sec). Value will be negative for inflow, positive for outflow. (F10.0) | N, from flat file |
| **Record 4** | **Data Group Identification 20A4)** | |

**Table 6: DATA GROUP F: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| HEADER | alphanumeric characters to identify the type of inflows, "VARIABLE INFLOW DATA." (20A4) | N |
| **Record 5** | **Variable Inflow Number (I5)** | |
| NVFLOW | the number of variable inflows that will be read. (I5)<br>If NVFLOW = 0, skip to Data Group G. | N |
| **Record 6** | **Variable Inflow Breaks (2I10) -**<br>**Records 6 and 7 are repeated as a unit NVFLOW times.** | |
| JRVF(I) | junction that will be receiving the following variable inflows. (I10) | N |
| NINCR(I) | number of data points (breaks) for variable inflow into junction JRVF(I). (I10) | N |
| **Record 7** | **Variable Inflow Data (4(F5.0, F3.0, F2.0, F10.0))** | |
| DAY(K) | day of VFLOW(I,K) (day). (F5.0) | N |
| HR(K) | hour of VFLOW(I,K) (hr). (F3.0) | N |
| MIN(K) | minute of VFLOW(I,K) (min). (F2.0) | N |
| VFLOW(I,K) | value of the variable flow corresponding to DAY(K), HR(K), and MIN(K) (m3/ sec). Value will be negative for inflow, positive for outflow. (F10.0) | N |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.7 Data Group G: Seaward Boundary Data

**Table 7: DATA GROUP G: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (20A4)** | |
| HEADER | alphanumeric characters to identify the data group, "SEAWARD BOUNDARY DATA." (20A4) | enter: "Seaward Boundary Data" |
| **Record 2** | **Seaward Boundary Number (I5)** | |
| NSEA | number of seaward boundaries on model network. (I5)<br>If NSEA = 0, skip to Data Group H. | NSEA = 0 |
| **Record 3** | **Seaward Boundary Parameters (4I5, 4F5.0)** | |

## Table 7: DATA GROUP G: RECORD FORMAT

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| SEAOPT | Seaward boundary input option (I5): 1: input regression coefficients for single tidal cycle; 2: input height versus time for single tidal cycle; 3: enter high and low tidal heights versus time for multiple tidal cycles. (I5)<br>• If SEAOPT = 2, height versus time data for a single tidal cycle will be fit to the following regression:<br><br>Head = A1(J,1) + A2(J,2) sin(?t) + A3(J,3) sin(2?t) + A4(J,4) sin(3?t) + A5(J,5) cos(?t) + A6(J,6) cos(2?t) + A7(J,7) cos(3?t)<br><br>• If SEAOPT = 3, tidal highs and lows will be fit to half sine curves.<br>• If SEAOPT = 1, use Records 4.1 and 5.1 => coefficients for average tide are given.<br>• If SEAOPT = 2, use Records 4.2 and 5.2 => calculates coefficients for average tide.<br>• If SEAOPT = 3, use Record 4.3 => variable tide is calculated. | N/A |
| JJ | junction number receiving the tidal input. (I5) | N/A |
| NDATA | number of data points (or breaks) used to describe the seaward tide (I5). | N/A |
| MAXIT | maximum number of iterations allowed to calculate average tide. (I5) | N/A |
| MAXRES | maximum error allowed in calculation of average tide (calculates coefficients to describe tidal cycle). (F5.0) | N/A |
| TSHIFT | allows tidal cycle to be shifted on the time scale. Therefore, if all data have been entered and error of 6.5 hours has been made in time scale, one can enter 6.5 for TSHIFT (hr). Usually equal to zero. (F5.0) | N/A |
| PSHIFT | allows tidal cycle to be shifted on the phase angle scale (radians). Usually equal to zero. (F5.0) | N/A |
| YSCALE | scale factor for observed heads (F5.0): | N/A |
| Record 4.1 | Tidal Parameters (2F10.0) | N/A |
| PERIOD(J) | tidal period (hr). (F10.0) | N/A |
| TSTART(J) | starting time for tidal input (hr). (F10.0) | N/A |
| **Record 4.1** | **Coefficients (7F10.0) -**<br>These coefficients describe the curve with the following equation:<br>Head = A1(J,1) + A2(J,2) sin(?t) + A3(J,3) sin(2?t) + A4(J,4) sin(3?t) + A5(J,5) cos(?t) + A6(J,6) cos(2?t) + A7(J,7) cos(3?t) | |
| A1(J,1) | 1st Coefficient. (F10.0) | N/A |
| A1(J,2) | 2nd Coefficient. (F10.0) | N/A |
| A1(J,3) | 3rd Coefficient. (F10.0) | N/A |
| A1(J,4) | 4th Coefficient. (F10.0) | N/A |

**Table 7: DATA GROUP G: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| A1(J,5) | 5th Coefficient. (F10.0) | N/A |
| A1(J,6) | 6th Coefficient. (F10.0) | N/A |
| A1(J,7) | 7th Coefficient. (F10.0) | N/A |
| Record 4.2 | Tidal Parameters (2F10.0) | N/A |
| PERIOD(J) | tidal period (hr). (F10.0) | N/A |
| TSTART(J) | starting time for tidal input (hr). (F10.0) | N/A |
| **Record 4.2** | **Tidal Data (4(F5.0, 1XF20, F2.0, F10.0))** | |
| DAY(I) | day corresponding to BHEAD(I) (day). (F5.0) | N/A |
| HR(I) | hour corresponding to BHEAD(I) (hr). (F2.0) | N/A |
| MIN(I) | minute corresponding to BHEAD(I) (min) (F2.0) | N/A |
| BHEAD(I) | tidal elevation (head) at time DAY(I), HR(I), and MIN(I) (m). (F10.0) | N/A |
| **Record 4.3** | **Tidal Data (4(F5.0, 1XF20, F2.0, F10.0))** | |
| DAY(I) | day corresponding to BHEAD(I) (day). (F5.0) | N/A |
| HR(I) | hour corresponding to BHEAD(I) (hr). (F2.0) | N/A |
| MIN(I) | minute corresponding to BHEAD(I) (min) (F2.0) | N/A |
| BHEAD(I) | tidal elevation (head) at time DAY(I), HR(I), and MIN(I) (m). (F10.0) | N/A |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

As discussed above, three options for describing the tidal cycle exists: 1) give coefficients for average tide, 2) calculate coefficients for average tide, or 3) give highs and lows for variable tide. For all three options, records 1, 2, and 3 are entered once. For Option 1, Records 4.1 and 4.2 are entered once. For Option 2, Record 4.2 is entered once, and Record 5.2 is entered as many times as needed with 4 tidal elevations on each line. For Option 3, Record 4.3 is entered as many times as needed with 4 tidal elevations on each line.

## 3.8 Data Group H: Wind Data

**Table 8: DATA GROUP H: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (20A4) - (Records 1 and 2 are entered once)** | |

**Table 8: DATA GROUP H: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| HEADER | alphanumeric characters to identify the data group, "WIND DATA." (20A4) | P |
| **Record 2** | **Wind Data Number (I5)** | |
| NOBSW | number of wind data points (or breaks).<br>If NOBSW = 0, skip to Data Group I. | N |
| **Record 3** | **Wind Data (4(F5.0, 1X, F2.0, F2.0, 2F5.0)) -<br>(entered as many times as needed with 4 wind speeds on each line)** | |
| DAY(K) | day corresponding to the following wind speed and wind direction (day). (F5.0) | N |
| HR(K) | hour corresponding to the following wind speed and wind direction (hr). (F2.0) | N |
| MIN(K) | minute corresponding to the following wind speed and wind direction (min). (F2.0) | N |
| WINDS(K) | wind speed measured at a distance of 10 meters above the water system (m/ sec). (F5.0) | N |
| WDIR(K) | wind direction measured at a distance of 10 meters above the water system. Must be measured from True North (degrees). (F5.0) | N |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.9 Data Group I: Precipitation/evaporation Input

**Table 9: DATA GROUP I: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification Header (A80) -<br>(Record 1 and 2 are entered once)** | |
| HEADER | alphanumeric characters to identify the data group, "PRECIPITATION/ EVAPORATION DATA." (20A4) | enter: "Precipitation/ Evaporation Data." |
| **Record 2** | **Input Data description (I5, 2F10.0)** | |
| NOEVA | Number of Precipitation Data Points (I5)<br>If NOEVA = 0, skip to Data Group J. | N |
| SCALE | Scale Factor (F10.0) | P |
| CONVE | Units Conversion Factor (F10.0) | P |

**Table 9: DATA GROUP I: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 3** | **Precipitation/Evaporation Time Function (4(F5.0,1X,2F2.0,F10.0)) - four sets of data can be entered per line. If NOEVA = 0, skip to segment mapping.** | |
| DAY(K) | Day corresponding to rainfall event | N |
| HR(K) | Hour corresponding to rainfall event | N |
| MIN(K) | Minute corresponding to rainfall event | N |
| EVAP(K) | Precipitation/Evaporation Rate (M/SEC) for corresponding DAY(K),HR(K),MIN(K). If rainfall units are cm/day or cm/year the conversion factors are 1.157E-7 and 3.17E-10. NOTE: Precipitation is positive, evaporation is negative. | N |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.10 DATA GROUP J: JUNCTION GEOMETRY INPUT DATA

**Table 10: DATA GROUP J: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (A80) - (Record 1 and 2 are entered once)** | |
| HEADER | alphanumeric characters to identify the data group, "VARIABLE JUNCTION GEOMETRY DATA." (20A4) | enter: "Variable Junction Geometry Data." |
| **Record 2** | **Number of junctions with Variable Surface Area (I5)** | |
| IJ | Number of Junctions with variable surface areas. (I5) If IJ = 0, skip to Data Group K. | N |
| **Record 3** | **Junction Geometry Data (JJ,SAN(JJ)) (I5, F10.0) - (entered IJ times)** | |
| JJ | Junction Number (I5) | N |
| SAN (JJ) | Ratio of change in surface area with respect to surface elevation (F10.0) | N |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.11 Data Group K: Channel Geometry Input Data

**Table 11: DATA GROUP K: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification (A80) - (Record 1 and 2 are entered once)** | |
| HEADER | alphanumeric characters to identify the data group, "VARIABLE CHANNEL GEOMETRY DATA." (20A4) | enter: "Variable Channel Geometry Data." |
| **Record 2** | **Number of Channels with Variable Width (I5)** | |
| IC | Number of Channels with variable width. (I5)<br>If IC = 0, skip to Data Group L. | S |
| **Record 3** | **Channel Geometry Data (I5,F10.0) - (entered ICC times)** | |
| ICC | Channel Number (I5) | S |
| SLOPE (ICC) | Ratio of change in channel width with respect to change in HEAD (F10.0).<br>Note: A value of zero implies a rectangular channel. | S |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 3.12 Data Group L: DYNHYD Junction To Wasp Segment Map

**Table 12:**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Group Identification Header (A80)** | |
| HEADER | alphanumeric characters to identify the data group, "JUNCTION TO SEGMENT MAP." (20A4) | enter: "Junction to Segment Map." |
| **Record 2** | **DYNHYD to WASP Linkage Options (2I5)** | |

**Table 12:**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| HDEPVEL | Switch controlling the writing of information to the interfacial hydrodynamic file for WASP (I5):<br>• 0 = DYNHYD will write time variant segment velocities and depths for WASP.<br>• 1 = DYNHYD will write one set of segment velocities and depths for WASP to read. Note: This option should be used in situations where depth and velocity are NOT changing radically. | P |
| NPAIR | Number of DYNHYD junctions to map to WASP5 segment network. (I5) | N |
| **Record 3** | **DYNHYD Junction to WASP Segment Map (2I5)** | |
| JUNSEG(J) | Junction number to map out for WASP input. (I5) | N |
| WASPSEG(J) | WASP segment to receive the flow data from JUNSEG. (I5)<br>This option allows the user to map portions of the DYNHYD output for WASP. | N |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

# 4.0 WASP Inputs by Card

## 4.1 Overview

This section describes the 10 data groups supported by WASP 5 (Ambrose et al., 1993), these data groups support the three modules in WASP 5 (EUTRO, TOXI, and META):

- A - Model Identification and Simulation Control, the number of segments, number of systems, time step, and print intervals are specified in this group.
- B - Exchange Coefficients, contains dispersive exchange information between segments and along characteristic lengths which may vary in time and linearly along segments.
- C - Volumes, supplies the initial segment volume, type, and underlying number information. Hydraulic geometry information can be give such as average depth and velocity as a function of flow. These data are used in the recreation and volatilization calculations and not the basic transport equations.
- D - Flows, supplies flow and sediment transport information between segments at each boundary. An external file may be used to supply flow data.
- E - Boundary Concentrations, boundary concentrations for each segment boundary. These may vary in a piecewise linear time function.
- F - Waste Loads, defines waste loads for point and diffuse sources. Point sources may vary in a piecewise linear time function and nonpoint sources may vary with time in a daily step function.
- G - Environmental Parameters, contains environmental characteristics of the water body for each segment.
- H - Chemical Constants, contains appropriate chemical characteristics of constants, these remain consistent in time and space.
- I - Time Functions, appropriate environmental or kinetic time functions.
- J - Initial Conditions, contains the initial concentration for each segment and each system along with the dissolved fractions and density of solids systems.

## 4.2 EUTRO4 Eutrophication Model

The eutrophication model (EUTRO4) requires the same input format as the basic WASP5 model, but

requires specific variables, see *Table 13*.

**Table 13: EUTRO4 Systems of Complexity[a]**

| System Number | Symbol | Name | Use in Complexity Level | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | 1[b] | 2[c] | 3[d] | 4[e] | 5[f] | 6[g] |
| 1 | $NH_3$ | Ammonia nitrogen | | ✔ | ✔ | ✔ | ✔ | ✔ |
| 2 | $NO_3$ | Nitrate nitrogen | | | ✔ | ✔ | ✔ | ✔ |
| 3 | $PO_4$ | Inorganic phosphorus | | | | ✔ | ✔ | ✔ |
| 4 | CHL | Phytoplankton carbon | | | | ✔ | ✔ | ✔ |
| 5 | CBOD | Carbonaceous BOD | ✔ | ✔ | ✔ | ✔ | ✔ | ✔ |
| 6 | DO | Dissolved oxygen | ✔ | ✔ | ✔ | ✔ | ✔ | ✔ |
| 7 | ON | Organic nitrogen | | | ✔ | ✔ | ✔ | ✔ |
| 8 | OP | Organic phosphorus | | | | ✔ | ✔ | ✔ |

a. Adapted from Ambrose (1993) page 3.
b. "Streeter-Phelps" BOD-DO with SOD
c. "Modified Streeter-Phelps" with NBOD
d. Linear DO balance with nitrification
e. Simple eutrophication
f. Intermediate eutrophication
g. Intermediate eutrophication with benthos

The complexity levels in *Table 13* are suggestions, any combination of variables can be selected by the user.

## 4.3 TOXI4 - Toxic Chemical Model

The toxic chemical model (TOXI4) requires the same input format as the basic WASP5 model, with the specific variables as described in *Table 14*.

**Table 14: TOXI4 Systems and Levels of Complexity[a]**

| System Number | Symbol | Name | Levels of Complexity for Solids | | | Levels of Complexity for Kinetics | |
|---|---|---|---|---|---|---|---|
| | | | 1, 2[b] | 3[c] | 4[d] | 1-3[e] | 4[f] |
| 1 | $C_1$ | Chemical 1 | ✔ | ✔ | ✔ | ✔ | ✔ |
| 2 | $S_1$ | Solid 1 | | ✔ | ✔ | | |
| 3 | $S_2$ | Solid 2 | | | ✔ | | |

**Table 14: TOXI4 Systems and Levels of Complexity[a]**

| System Number | Symbol | Name | Levels of Complexity for Solids | | | Levels of Complexity for Kinetics | |
|---|---|---|---|---|---|---|---|
| 4 | $S_3$ | Solid 3 | | | ✔ | | |
| 5 | $C_2$ | Chemical 2 | | | | | ✔ |
| 6 | $C_3$ | Chemical 3 | | | | | ✔ |

a. Adapted from Ambrose (1993) page 5.
b. Solids 1, 2 - descriptive solids concentration field, with specific solid transport rates for solids 2.
c. Solids 3 - simulated total solids
d. Solids 4 - Three simulated solids types
e. Kinetic 1-3 - constant half lives or rated constants, spatially-variable rate constants, and second order rates respectively.
f. Kinetic 4 - Transformation products

The levels of complexity in *Table 14* are suggestive, the user may choose to simulate any combination of these variables.

## 4.4 META4 - Metals Model

This model contains the kinetics describing the fate of toxic metals in an aquatic environment. It models total metal concentrations for four different metals including Cd+2, Zn+2, Pb+2 and Mn and up to 3 classes of solids. The distribution of each form of the metal between the dissolved and various particulate phases is computed from the total concentration based on speciation and partitioning to solid phases.

The total concentration for each toxic metal includes dissolved chemical, chemical adsorbed to dissolved organic carbon and chemical adsorbed to the solids, i.e.,

```
Total Concentration = Dissolved + Reversibly Sorbed to Solids
 + Reversibly sorbed to Dissolved Organic Carbon
```

**Table 15: META4 - Metals Model**

| System Number | Symbol | Name |
|---|---|---|
| 1 | Cd (+2) | Cadmium |
| 2 | Zn (+2) | Zinc |
| 3 | Pb (+2) | Lead |
| 4 | Mn | Managanese |
| 5 | SOLIDS 1 | User Specified |
| 6 | SOLIDS 2 | User Specified |
| 7 | SOLIDS 3 | User Specified |
| NOSYS +1 | H(-) | Hydrogen Ion |

**Table 15: META4 - Metals Model**

| System Number | Symbol | Name |
|---|---|---|
| NOSYS +2 | $CO_3$ (-2) | Carbonate |
| NOSYS +3 | DOC | Dissolved Organic Carbon |
| NOSYS +4 | Ca (+2) | Calcium |
| NOSYS +5 | $SO_4$ | Sulfate |
| NOSYS +6 | Mg (+2) | Magnesium |

## 4.5 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. The Group A input data contains most of the general options that define a WASP5 run. The user must select the eutrophication, toxics, or metals option and appropriate state variables).

**Table 16: DATA GROUP A: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Title of Simulation (A5, A75)** | |
| SIMTYP | Simulation Type (A5) -<br>TOXI4 = toxics dataset<br>EUTRO = eutrophication dataset<br>METALS = metals dataset | P |
| TITLE1 | descriptive title of simulation. (A75) | P |
| **Record 2** | **Description of Simulation (A80)** | |
| TITLE2 | description of simulation. (A80) | P |
| **Record 3** | **Record 4 Names (A80)** | |
| HEADER | names of Record 4 variables, positioned properly; for user convenience only. (A80) | P |
| **Record 4** | **Simulation Control Parameters (7I5, 2F5.0, F3.0, F2.0)** | |
| NOSEG | number of segments in model network. (I5) | P |
| NOSYS | number of model systems (state variables). (I5) | P |

## Table 16: DATA GROUP A: RECORD FORMATS

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| 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) | P |
| MFLAG | flag controlling messages printed on screen during simulation; 0 = all messages printed; 1 = simulation time only printed; 2 = all messages are suppressed. (I5) | T, P |
| JMASS | system number for which mass balance analysis will be performed; 0 = no mass balance table generated. (I5) | P |
| NEGSLN | negative solution option; 0 = prevents negative solutions; 1 = allows negative solutions. (I5) | P |
| INTYP | time step option; 0 = user inputs time step history; 1 = model calculates time step. (I5) | P |
| ADFAC | advection factor; 0 = backward difference; 0.5 = central difference; 0-0.4 recommended. (F5.0) | P |
| ZDAY | day at beginning of simulation; 1 is first day. (F5.0) | T, P |
| ZHR | hour at the beginning of simulation. (F3.0) | T, P |
| ZMIN | minute at the beginning of simulation. (F2.0) | T, P |
| TFLG | switch controlling generation of transport file; 0 = generate file; 1 = do not generate file. (I5) | P |
| **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) | P |
| **Record 6** | **Number of Time Steps (I5)** | |
| NOBRK | number of different model time steps (I5) | T, P |
| Record 7 | Time Steps (4(F10.0, F10.0)) | T, P |
| DTS(I) | time step to be used until time T(I), days. (F10.0) | T, P |
| T(I) | time up to when time step DTS(I) will be used, days. (F10.0) | T, P |
| **Record 8** | **Number of Print Intervals (I5)** | |
| NPRINT | number of print intervals. (I5) | T, P |
| **Record 9** | **Print Intervals (4(F10.0, F10.0))** | |

**Table 16: DATA GROUP A: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| PRINT(I) | print interval to be used until time TPRINT(I), days. (F10.0) | T, P |
| TPRINT(I) | time up to when print interval PRINT(I) will be used, days. (F10.0) | T, P |
| **Record 10** | **System Bypass Options (16I5)** | |
| SYSBY(K) | bypass option for system K; 0 = system will be simulated; 1 = system will be bypassed. (I5) | P |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 4.6 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.

**Table 17: DATA GROUP B: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Number of Exchange Fields (I5, 75X)** | |
| NRFLD | 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. | P |
| TITLE | name of data group. (75X) | enter: "Exchange Fields." |
| **Record 2** | **Exchange Time Functions for Surface Water Field (I5, 2F10.0)** | |
| NTEX(1) | number of exchange time functions for field 1. (I5)<br>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). | P |
| SCALR | scale factor for exchange coefficients. All exchange coefficients for field 1 will be multiplied by this factor. (F10.0) | P |
| CONVR | conversion factor for exchanges in field 1. (F10.0) | P |
| **Record 3** | **Exchange Data (I5) - (input NTEX(1) times)** | |

## Table 17: DATA GROUP B: RECORD FORMATS

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| NORS(1,NT) | number of exchanges for field 1, time function NT. (I5) | P |
| **Record 4** | **Areas, Characteristic Lengths (2F10.0, 2I5) - (repeated NORS(1,NT) times)** | |
| A(K) | area in square meters for exchange pair K. (F10.0) | P |
| EL(K) | characteristic length in meters for exchange pair K. (F10.0) | P |
| IR(K),JR(K) | segments between which exchange occurs. The order of the segments is unimportant. (2I5) | P |
| **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) | T, P |
| **Record 6** | **Piecewise Linear Dispersion Time Function (4(F10.0, F10.0)) - (repeated NBRKR(1,NT)/4 times)** | |
| RT(K) | value of dispersion coefficient in m2/sec at time TR(K). (F10.0) | T, P |
| TR(K) | time in days. (F10.0) | T, P |
| **Record 7** | **Exchange Time Functions for Pore Water Field (I5, 2F10.0)** | |
| NTEX(2) | number of exchange time functions for field 2. (I5)<br>To skip pore water exchange field, set NTEX(2) to zero and continue with record 12. | P |
| SCALR | scale factor for exchange coefficients. All exchange coefficients for field 2 will be multiplied by this factor. (F10.0) | P |
| CONVR | conversion factor for exchanges in field 2. (F10.0) | P |
| **Record 8** | **Exchange Data (I5) - (Records 8-11 are input as a group NTEX(2) times)** | |
| NORS(2,NT) | number of exchanges for field 2, time function NT. (I5)<br>NT = 1, NTEX(2) | P |
| **Record 9** | **Areas, Characteristic Lengths (2F10.0, 2I5) - (repeated NORS(2,NT) times)** | |
| A(K) | area in square meters for exchange pair K. (F10.0) | P |
| EL(K) | characteristic length in meters for exchange pair K. (F10.0) | P |
| IR(K),JR(K) | segments between which exchange occurs. The order of the segments is unimportant. (2I5) | N |

**Table 17: DATA GROUP B: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **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) | T, P |
| **Record 11** | **Piecewise Linear Dispersion Time Function (4(F10.0, F10.0)) - (repeated NBRKR(2,NT)/4 times)** | |
| RT(K) | value of dispersion coefficient in m2/sec at time TR(K). (F10.0) | T, P |
| TR(K) | time in days. (F10.0) | T, P |
| **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)<br>K = 1, NOSYS | P |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

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.

## 4.7 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.

**Table 18: DATA GROUP C: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Preliminary Data (2I5, F10.0, 60X)** | |

**Table 18: DATA GROUP C: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| IVOPT | water column volume option<br>1 = constant water column volumes; 2, 3 = volumes adjusted to maintain flow continuity. (I5) | P |
| IBEDV | benthic volume option<br>0 = constant bed volumes; 1, bed volumes change in response to sediment transport. (I5) | P |
| TDINTS | benthic time step in days for recomputing porosity (if IBEDV = 0) or for sediment bed compaction (if IBEDV = 1). (F10.0) | P |
| TITLE | name of data group. (60X) | enter: "Preliminary Data." |
| **Record 2** | **Scale Factors (2F10.0)** | P |
| SCALV | scale factor for volumes. All volumes will be multiplied by this factor. (F10.0) | P |
| CONVV | conversion factor for volumes. (F10.0) | P |
| **Record 3** | **Segment Types and Volumes (3I10, 5F10.0)<br>(repeated NOSEG times)** | |
| ISEG | segment number. | S |
| IBOTSG | segment immediately below ISEG. (I10) | N |
| ITYPE(ISEG) | segment types: 1 = surface water segment, 2 = subsurface water segment, 3 = upper bed segment, 4 = lower bed segment. (I10) | S |
| BVOL(ISEG) | volume of segment ISEG in cubic meters. (F10.0) | S |
| VMULT(ISEG) | hydraulic coefficient "a" for velocity in ISEG as a function of flow:<br>v= a Qb, If b = 0, VMULT is a constant velocity in m/sec. (F10.0) | S |
| 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) | S |
| DMULT(ISEG) | hydraulic coefficient "c" for depth of ISEG as a function of flow:<br>d = c Qd, If d = 0, DMULT is a constant depth in m. (F10.0) | S |
| 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) | S |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

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.

## 4.8 Data Group D: Flows

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.

**Table 19: DATA GROUP D: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Input Options: Number of Flow Fields (2I5, A12)** | |
| NFIELD | number of flow fields.<br>• 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.<br>• 2 = field one flows are specified directly by the user. Individual flows at each segment interface are applied directly by the model<br>• 3 = flows are read from a formatted file created by DYNHYD5 or other hydrodynamic model. (I5)<br>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) | P |
| HYDFIL | name of hydrodynamic file to be read by WASP5 during the simulation (for example, RIVER1.HYD). (A12) | P<br>Note - this will be a file from DYNHYD |
| **DATA BLOCK D1:** | **Direct Input of Field One Flows (IQOPT = 1,2)** | |
| **Record 2** | **Number of Flow Time Functions (I5, 2F10.0) - (input once for Data Block D1)** | |
| 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) | T |
| SCALQ | scaling factor. All flows in Field one are multiplied by SCALQ. (F10.0) | P |
| CONVQ | units conversion factor. (F10.0) | P |

## Table 19: DATA GROUP D: RECORD FORMATS

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 3** | **Number of Flows (I5) - (Records 3 - 6 are input as a group NINQ(1) times, input once for each flow time function.)** | |
| 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) | N |
| **Record 4** | **Flow Routing for Field One (4(F10.0, 2I15)) - (repeated NOQS(1,NI)/4 times, as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets per line)** | |
| BQ(1,NI,K) | portion of flow for field one, time function NI that flows between segment pair K. (F10.0) | N |
| JQ(1,NI,K) | upstream segment. (I5) | N |
| IQ(1,NI,K) | downstream segment. (I5) | N |
| **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) | N, T |
| **Record 6** | **Piecewise Linear Advective Time Function (4(2F10.0)) - (repeated NBRKQ(1,NI) times, as many lines as necessary to input NBRKQ sets of QT and TQ, with four sets on each line)** | |
| QT(1,NI,K) | advective flow in m3/s. (F10.0) | T |
| TQ(1,NI,K) | time in days. (F10.0) | T |
| **DATA BLOCK D2:** | **Field Two (Pore Water) Flows** | |
| **Record 7** | **Number of Pore Water Time Functions (I5, 2F10.0) - (input once for Data Group D2)** | |
| 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) | N, T |
| SCALQ | scaling factor for pore water flows. (F10.0) | T |
| CONVQ | units conversion factor. (F10.0) | T |
| **Record 8** | **Number of Flows (I5) - (records 8 - 11 are input as a group NINQ(2) times, input once for each pore water time function)** | |
| NOQS(2,NI) | number of segment pair flows in Field 2, time function NI. (I5) | N |

**Table 19: DATA GROUP D: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 9** | **Flow Routing for Field Two (4(F10.0, 2I5)) - (Record 9 is repeated NOQS(2,NI)/4 times, as many lines as necessary to input NOQS sets of BQ, JQ, and IQ, with four sets on each line)** | |
| BQ(2,NI,K) | portion of pore water flow for time function NI that flows between segment pair K. (F10.0) | N, T |
| JQ(2,NI,K) | upstream segment. (I5) | N |
| IQ(2,NI,K) | downstream segment. (I5) | N |
| **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) | N |
| **Record 11** | **Piecewise Linear Velocity Time Function (4(2F10.0)) - (repeated NBRKQ(2,NI)/4 times, as many lines as necessary to input NBRKQ sets of QT and TQ, with four sets on each line)** | |
| QT(2,NI,K) | pore water flow in m3/s. (F10.0) | S |
| TQ(2,NI,K) | time in days. (F10.0) | N, T |
| **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) - (input once for Data Block D3)** | |
| NINQ(3) | number of velocity time functions for Field 3. (I5) | T |
| SCALQ | scaling factor for velocities. (F10.0) | P |
| CONVQ | units conversion factor. (F10.0) | P |
| **Record 13** | **Number of Segment Pairs (I5) - (Records 13 - 16 are input as a group NINQ(3) times, input for each velocity time function)** | |
| NOQS(3,NI) | number of segment pairs involved in sediment 1 transport. (I5) | N |
| **Record 14** | **Areas for Settling, Resuspension (4(F10.0, 2I5)) - (repeated NOQS(3,NI)/4 times, as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line)** | |

**Table 19: DATA GROUP D: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| BQ(3,NI,K) | area in square meters between segment pair K. (F10.0) | N |
| JQ(3,NI,K) | segment sediment is transported from. (I5) | N |
| IQ(3,NI,K) | segment sediment is transported to. (I5) | N |
| **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) | T |
| **Record 16** | **Piecewise Linear Velocity Time Function (4(2F10.0)) (repeated NBRKQ(3,NI)/4 times, as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line)** | |
| QT(3,NI,K) | sediment 1 transport velocity in m/s. (F10.0) | N |
| TQ(3,NI,K) | time in days. (F10.0) | N |
| **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) (input once for Data Block D4)** | |
| NINQ(4) | number of velocity time functions for Field 4. (I5) | T |
| SCALQ | scaling factor for velocities. (F10.0) | P |
| CONVQ | units conversion factor. (F10.0) | P |
| **Record 18** | **Number of Segment Pairs (I5) - (records 18 - 21 are input as a group NINQ(4) times, input for each velocity time function)** | |
| NOQS(4,NI) | number of segment pairs involved in sediment 2 transport. (I5) | N |
| **Record 19** | **Areas for Settling, Resuspension (4(F10.0, 2I5)) - (repeated NOQS(4,NI)/4 times, uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line.)** | |
| BQ(4,NI,K) | area in square meters between segment pair K. (F10.0) | N |
| JQ(4,NI,K) | segment sediment is transported from. (I5) | N |
| IQ(4,NI,K) | segment sediment is transported to. (I5) | N |

**Table 19: DATA GROUP D: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **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) | T |
| **Record 21** | **Piecewise Linear Velocity Time Function (4(2F10.0)) - (repeated NBRKQ(4,NI)/4 times, uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line)** | |
| QT(4,NI,K) | sediment 2 transport velocity in m/s. (F10.0) | T |
| TQ(4,NI,K) | time in days. (F10.0) | T |
| **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) - (input once for Data Block D5)** | |
| NINQ(5) | number of velocity time functions for Field 5. (I5) | T |
| SCALQ | scaling factor for velocities. (F10.0) | P |
| CONVQ | units conversion factor. (F10.0) | P |
| **Record 23** | **Number of Segment Pairs (I5) (Records 23 - 26 are input as a group NINQ(5) times, input for each velocity time function.)** | |
| NOQS(5,NI) | number of segment pairs involved in sediment 3 transport. (I5) | N |
| **Record 24** | **Areas for Settling, Resuspension (4(F10.0, 2I5)) - (Record 24 is repeated NOQS(5,NI)/4 times, uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line)** | |
| BQ(5,NI,K) | area in square meters between segment pair K. (F10.0) | N |
| JQ(5,NI,K) | segment sediment is transported from. (I5) | N |
| IQ(5,NI,K) | segment sediment is transported to. (I5) | N |
| **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) | T |

## Table 19: DATA GROUP D: RECORD FORMATS

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 26** | **Piecewise Linear Velocity Time Function (4(2F10.0)) - (record 26 is repeated NBRKQ(5,NI)/4 time, uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.)** | |
| QT(5,NI,K) | sediment 3 transport velocity in m/s. (F10.0) | P |
| TQ(5,NI,K) | time in days. (F10.0) | P |
| **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) | T |
| SCALQ | scaling factor for velocities. (F10.0) | P |
| CONVQ | units conversion factor. (F10.0) | P |
| **Record 28** | **Number of Segment Pairs (I5) - (Records 28 - 31 are input as a group NINQ(6) times)** | |
| NOQS(6,NI) | number of segment pairs involved in evaporation or precipitation. (I5) | N |
| **Record 29** | **Areas for Evaporation, Precipitation (4(F10.0, 2I5)) - (repeated NOQS(6,NI)/4 times)** | |
| BQ(6,NI,K) | area in square meters between segment pair K. (F10.0) | N |
| JQ(6,NI,K) | segment water is transported from; if = 0, this is precipitation. (I5) | N |
| IQ(6,NI,K) | segment water is transported to; if = 0, this is evaporation. (I5) | N |
| **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) | T |
| **Record 31** | **Piecewise Linear Velocity Time Function (4(2F10.0)) - (repeated NBRKQ(6,NI)/4 times)** | |

**Table 19: DATA GROUP D: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| 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) | P |
| TQ(6,NI,K) | time in days. (F10.0) | T |
| **END OF DATA BLOCKS FOR D** | | |
| **Record 32** | **Flow Bypass Options (16I5)** | |
| QBY(ISYS) | flow bypass option<br>• 0 = flow transport occurs in system ISYS<br>• 1 = flow transport is bypassed for system ISYS. (I5)<br>• ISYS = 1, NOSYS | P |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

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.

## 4.9 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:

**Table 20: EXTERNAL HYDRODYNAMIC FILE: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Options (2I5, 3F20.0, I5) - (input once)** | |
| NQSEG | Number of segments connected by flows from the hydrodynamic file. (I5) | S |
| NQINT | Number of interfacial flow pairs from the hydrodynamic file. (I5) | N |
| DELTQ | WASP5 time step; an even multiple of the hydrodynamic time step, seconds. (F20.0) | T |

**Table 20: EXTERNAL HYDRODYNAMIC FILE: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| TBEGIN | Beginning time for the hydrodynamic file, in seconds. (F20.0) | T |
| TEND | Ending time for the hydrodynamic file, in seconds. (F20.0) | T |
| 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) | P |
| **Record 2** | **Segment Interface Pairs (2I5) - (repeated NQINT times, for J from 1 to NQINT)** | |
| IQ(J) | First segment in interface "J", nominally where flow is from. (I5) | S |
| 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. | S |
| **Record 3** | **Initial Segment Properties (4F20.0) - (repeated NQSEG times, for I from 1 to NQSEG)** | |
| BVOL(I) | Volume of segment "I" at beginning of time step, m3. (F20.0) | S |
| DUMMY | Dummy variable, not used by WASP5. (20.0) | S |
| DEPTH(I) | Average depth of segment "I", in meters. (F20.0) | S |
| VELOC | Average velocity of segment "I", m/sec. (F20.0) | S |
| **Record 4** | **Segment Interfacial Flows (F20.0) - (Records 4 and 5 are repeated as a unit for the number of time steps in the water quality simulation, or NQINT times, for J from 1 to NQINT (in the same order as segment pairs are given in Record 2) (TEND - TBEGIN)/DELTQ.)** | |
| BQ(J) | Average flow in interfacial pair "J" during the time step, in $m^3$/sec. (F20.0) | N |
| **Record 5** | **Segment Properties (4F20.0) - (repeated NQSEG times, for I from 1 to NQSEG)** | |
| BVOL(I) | Volume of segment "I" at end of time step, m3. (F20.0) | S |
| DUMMY | Dummy variable, not used by WASP5. (20.0) | S |
| DEPTH(I) | Average depth of segment "I", in meters. (F20.0) | S |
| VELOC | Average velocity of segment "I", m/sec. (F20.0) | S |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 4.10 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.

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

**Table 21: DATA GROUP E: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Input Option - Number of Boundary Conditions (I10, 70X) - (Records 1, 2, and 3 are entered once. 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.)** 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. | |
| NOBC(K) | number of boundary conditions used for system K. (I10) | |
| TITLE | name of data group. (70X) | enter: "Boundary Concentrations." |
| **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) | P |
| CONVB | unit conversion factor for boundary conditions. Boundary conditions are expected to be in mg/L (i.e. - g/m3), in which case CONVB will be 1.0. (F10.0) | P |
| **Record 3** | **Boundary Location (2I5) - input as a unit NOBC(K) times:** | |
| IBC(K) | boundary segment number. (I5) | S |
| 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) | T |
| **Record 4** | **Boundary Concentrations (4(2F10.0)) - (repeated NOBRK(K)/4 times until NOBRK entries are input)** | |
| BCT(K) | value of the boundary concentration at time T(K) in mg/L. (F10.0) | T |
| 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) | T |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

### 0.0.1 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 mg/L. These are transformed internally to phytoplankton carbon using the carbon to chlorophyll ratio, which is specified in Data Group H as constant 46.

### 0.0.2 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 mg/L.)

## 4.11 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.

**Table 22: DATA GROUP F: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Number of Point Source Loadings (I10, 70X) - (records 1-4 is repeated in its entirety NOSYS times, records 1 and 2 are input once for each system)** 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. | |
| NOWK(ISYS) | Number of point source loadings used for system ISYS. (I10) 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. 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. | N |
| TITLE | name of data group. (70X) | enter: "Waste Loads." |
| **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) | P |

**Table 22: DATA GROUP F: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| 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) | P |
| **Record 3** | **Number of Point Sources (2I5) - (Records 3-4 are input as a unit NOWK(ISYS) times, within each set, Record 3 is entered once)** | |
| IWK(K) | segment number that has point source loading BWK(K). (I5) | S |
| 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) | S |
| **Record 4** | **Point Source Time Function (4(2F10.0)) - (repeated NOBRK(ISYS)/4 times)** | |
| WKT(K) | value of the point source loading at time T(K), in kg/day. (F10.0) | N |
| 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) | T |
| **Record 5** | **Nonpoint Source Load Option (I10) - (input once)** | |
| 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) | P |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

## 4.12 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.

**Table 23: EXTERNAL NONPOINT SOURCE FILE: RECORD FORMAT**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Data Options (A15, 3I5) - (input once)** | |
| NPSMOD | Name or description of nonpoint source model or method of generation; this is echoed to the output file for the record. (A15) | enter non-point source file name |
| NUMSEG | Number of segments receiving nonpoint source loads. (I5) | S |
| INTOPT | Interpolation option; 1 = step function (only one in code now). (I5) | P |
| NUMSYS | Number of WASP systems receiving nonpoint source loads. (I5) | P |
| **Record 2** | **Loading Segments (I5) - (repeated NUMSEG times)** | |
| LSEG(I) | segment number receiving loads. (I5) | S |
| **Record 3** | **Loading Systems (20I5) (input once)** | |
| LSYS(I) | WASP system numbers receiving loads. (I5) | P |
| **Record 4** | **System Descriptors (A15) - (repeated NUMSYS times)** | |
| NAMESY(I) | Name or description of WASP systems receiving loads. (A15) | P |
| **Record 5** | **Loading Days (F10.0) - (Records 5 and 6 are repeated as a unit for the number of days that nonzero loads occur, NUMSYS times)** | |
| LDAY | Time in days for the following nonzero load. (F10.0) | T |
| **Record 6** | **Nonpoint Source Loads (A15, 20F10.0) - (repeated NUMSYS times)** | |
| NAMESY(I) | System name or description (not read in by WASP). (A15) | P |
| 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) | S |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

### 0.0.3 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.

### 0.0.4 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.

## 4.13 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.

**Table 24: DATA GROUP G: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Number of Parameters (I10, 70X) - (input once)** | |
| 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) | P |
| TITLE | name of data group. (70X) | enter: "Parameters." |
| **Record 2** | **Scale Factors for Parameters (4(A5, I5, F10.0)) - (repeated NOPAM/4 times, Record 2 uses as many 80-space lines as needed to enter all NOPAM entries)** | |
| ANAME(ISC) | descriptive name for parameter ISC. (A5) | P |
| ISC | parameter number identifying parameter. (I5) | P |
| PSCAL(ISC) | scale factor for parameter ISC. (F10.0) | P |
| **Record 3** | **Segment Number (I10) (Records 3-4 are input as a unit NOSEG times, once for each segment.)** | |
| ISG | segment number for the following parameter values. (I10) | S |
| **Record 4** | **Segment Parameters (4(A5, I5, F10.0)) - (repeated NOPAM/4 times, uses as many lines as needed to enter all NOPAM entries)** | |
| PNAME(ISC) | an optional one to five alphanumeric character descriptive name for parameter PARAM(ISG,ISC). (A5) | P |
| ISC | parameter number identifying parameter. (I5) | P |

**Table 24: DATA GROUP G: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| PARAM (ISEG,ISC) | the value of parameter ISC in segment ISG. (F10.0) | S |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

### 0.0.5 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.

**Table 25: Parameters Available for EUTRO4 Simulations**

| ISC | NAME | 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/m2-day). |
| 8 | FPO4 | Average phosphate flux multiplier for segment (mg/m2-day). |
| 9 | SOD1D | Sediment oxygen demand for segment (g/m2-day). |
| 10- | RLGHTS | Used internally; not specified by the user. |

**Table 25: Parameters Available for EUTRO4 Simulations**

| ISC | NAME | Definition and Units |
|---|---|---|
| 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. |

### 0.0.6 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.

**Table 26: Parameters Used by TOXI4**

| ISC | NAME | Definition, Units, and Reactions Affected[a] |
|---|---|---|
| 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 (°C); 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 O3 for H2O2 (moles/L); O. |

**Table 26: Parameters Used by TOXI4**

| ISC | NAME | Definition, Units, and Reactions Affected[a] |
|---|---|---|
| 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. |
| 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). |

a. 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 20×C, 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 reareation 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.

## 4.14 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.

**Table 27: DATA GROUP H: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Header (80X) - (entered once)** | |
| TITLE | name of data group. (80X) | enter: "Constants." |
| **Record 2** | **Data Fields in Group ISYS (A10, I10) - (Records 2-4 are input as a group NOSYS+1 times)** | |
| CHNAME (ISYS) | a ten-character descriptive name for System (ISYS). (A10) | P |
| 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. | P |
| **Record 3** | **Number of Constants in Field (A10, I10) - (Records 3 and 4 are entered NFLD times)** | |
| FLDNAME | ten-character name identifying field of constants. (A10) | P |
| NCONS | number of constants to be entered in this field; 0 = no constants for this field (skip to next field). (I10) | P |
| **Record 4** | **Constants (2(A10, I10, F10.0)) - (repeated NCONS/2 times, NCONS entries (2 per line))** | |
| TNAME(ISC) | name identifying constant ISC. (A10) | P |
| ISC | number identifying constant; these numbers are set by model developer. (I10) | P |
| CONST(ISC) | value of constant ISC. (F10.0) | P |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

### 0.0.7 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.

**Table 28: Constants for Full Eutrophication Simulation**

| ISC | NAME | Definition and Units |
|---|---|---|
| 11 | K12C | Nitrification rate at 20×C, per day. |

**Table 28: Constants for Full Eutrophication Simulation**

| ISC | NAME | Definition and Units |
|---|---|---|
| 12 | K12T | Temperature coefficient for K1320C. Default = 1.0. |
| 13 | KNIT | Half-saturation constant for nitrification-oxygen limitation, mg O2/L. |
| 21 | K20C | Denitrification rate at 20×C, per day. |
| 22 | K20T | Temperature coefficient for K140C. Default = 1.0. |
| 23 | KNO3 | Half-saturation constant for denitrification oxygen limitation, mgO2/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 chla/ m3)-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:<br>• KMNG1 = 0, PNH3G1 = 1.0<br>• KMNG1 = Large, PNH3G1 = NH3/(NH3 + NO3)<br>NOTE: For standard model application, use a large KMNG1. |
| 49 | KMPG1 | Phosphorous half-saturation constant for phytoplankton growth, mg PO4-P/L. |
| 50 | K1RC | Endogenous respiration rate of phytoplankton at 20×C, 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 20×C, 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. |

**Table 28: Constants for Full Eutrophication Simulation**

| ISC | NAME | Definition and Units |
|---|---|---|
| 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 20×C, 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 20×C, 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 O2/mg C. Default = 32/12. |
| 82 | K2 | Reaeration rate constant at 20×C 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 20×C, 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 20×C, 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. |

### 0.0.8 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 29: CONSTANTS FOR SIMPLE TOXI4 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 111 | 711 | 1311 | PIXC(1,1) | Constant partition coefficient for sorption to solids (class 1), lw/kgs |
| | | | Ki: | 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 |

**Table 29: CONSTANTS FOR SIMPLE TOXI4 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 571 | 1171 | 1771 | KE | Extra reaction |
| | | | THi | 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 30: GENERAL CHEMICAL CONSTANTS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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, Lo/Lw |

**Table 31: IONIZATION CONSTANTS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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) | |

**Table 31: IONIZATION CONSTANTS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 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*TR/(T-TR)] |
| 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, °C |

**Table 32: SORPTION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 84 | 684 | 1284 | LKOW | Log 10 of the octanol-water partition coefficient, log (Lw/Lo) |
| 101 | 701 | 1301 | LKOC | Log 10 of the organic carbon partition coefficient, log (Lw/kgoc) |
| 102 | 702 | 1302 | A0 | Intercept in the Kow - Koc correlation: log Koc = A0 · log Kow; default = log 0.6 |
| 103 | 703 | 1303 | A1 | Slope in the Kow - Koc correlation; default = 1.0 |
| 106 | 706 | 1306 | NUX(1) | Solids-dependent partitioning parameter ($\upsilon x$) of the chemical onto solids; default = 1012 makes Kp independent of solids concentration |
| 111 | 711 | 1311 | PIXC(1,1) | Solids-independent (limiting) partition coefficient Kpo for sorption to solid 1, Lw/kgs |

**Table 32: SORPTION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 116 | 716 | 1316 | PIXC(2,1) | Solids-independent (limiting) partition coefficient Kpo for sorption to solid 2, Lw/kgs |
| 121 | 721 | 1321 | PIXC(3,1) | Solids-independent (limiting) partition coefficient Kpo for sorption to solid 3, Lw/kgs |
| | | | | If = 0, Kpo 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 33: LOCATION OF IONIC SORPTION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 |

**Table 33: LOCATION OF IONIC SORPTION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Ionic Specie** | **Sorptive Phase** |
| 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 34: VOLATILIZATION CONSTANTS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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-m3/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;<br>1 = stagnant pond or lake) |
| 5 | 5 | 5 | AIRTMP | Multiplier for air temperature time function |
| 8 | 608 | 1208 | ATMOS | Atmospheric concentration of chemical, µg/L |

**Table 35: SECOND ORDER BIODEGRADATION CONSTANTS FOR TOTAL FOR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 146 | 746 | 1346 | KBIO20(1,1) | Second-order 20°C 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 10°C temperature increase |
| 166 | 766 | 1366 | Q10DOC(1) | |
| 171 | 771 | 1371 | Q10PAR(1) | |

**Table 36: LOCATION OF IONIC BIODEGRADATION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 |

**Table 36: LOCATION OF IONIC BIODEGRADATION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Ionic Specie** | **Sorptive Phase** |
| 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 37: SECOND ORDER ALKALINE HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 184 | 784 | 1384 | TREFH | Reference temperature at which hydrolysis rates were measured, °C |
| 186 | 786 | 1386 | KH2O(1,1,1) | Second order, 20°C alkaline hydrolysis rate constants for aqueous, DOC-sorbed, and sediment-sorbed phases, L/mole-day |
| 191 | 791 | 1391 | KH2O(1,2,1) | |

**Table 37: SECOND ORDER ALKALINE HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 196 | 796 | 1396 | KH2O(1,3,1) | |
| 231 | 831 | 1431 | EHOH(1) | Activation energy for alkaline hydrolysis, kcal/mole |

**Table 38: LOCATION OF IONIC ALKALINE HYDROLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 39: SECOND ORDER NEURAL HYDROLYSIS CONSTANTS FOR TOTAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 184 | 784 | 1384 | TREFH | Reference temperature at which hydrolysis rates were measured, °C |
| 201 | 801 | 1401 | KH2O(2,1,1) | 20°C 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 40: LOCATION OF IONIC NEUTRAL HYDROLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 |

## Table 40: LOCATION OF IONIC NEUTRAL HYDROLYSIS CONSTANTS

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Ionic Specie** | **Sorptive Phase** |
| 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 41: SECOND ORDER ACID HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 184 | 784 | 1384 | TREFH | Reference temperature at which hydrolysis rates were measured, °C |
| 216 | 816 | 1416 | KH2O(3,1,1) | Second order, 20°C 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 42: LOCATION OF IONIC ACID HYDROLYSIS CONSTANTS

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 |

## Table 42: LOCATION OF IONIC ACID HYDROLYSIS CONSTANTS

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Ionic Specie** | **Sorptive Phase** |
| 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 43: SECOND ORDER OXIDATION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 258 | 858 | 1458 | TREFO | Reference temperature at which oxidation rates were measured, °C |
| 261 | 861 | 1461 | KOX2O(1,1) | Second-order, 20°C 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 44: LOCATION OF IONIC OXIDATION CONSTANTS

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 45: TOXI4 PHOTOLYSIS CONSTANTS

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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) |

## Table 45: TOXI4 PHOTOLYSIS CONSTANTS

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 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 |

## Table 46: GLOBAL CONSTANTS FOR TOXI4 PHOTOLYSIS OPTION 1

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 47: LOCATION OF IONIC PHOTOLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 |
| 559 | 1159 | 1759 | QUANTG(2,4) | - | B |

**Table 47: LOCATION OF IONIC PHOTOLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Ionic Specie** | **Sorptive Phase** |
| 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 48: EXTRA SECOND ORDER REACTIONS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 573 | 1173 | 1773 | TREFE | Reference temperature at which extra reaction rates were measured, °C |
| 576 | 1176 | 1776 | KE2O(1,1) | Second-order, 20°C 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 49: LOCATION OF IONIC EXTRA REACTION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **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 |

**Table 49: LOCATION OF IONIC EXTRA REACTION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Ionic Specie** | **Sorptive Phase** |
| 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 50: YIELD CONSTANTS FOR CHEMICAL 1 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| | | | Y()12: | Yield coefficient for production of C2 from C1, mgC2/mgC1 |
| 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 C3 from C1, mgC2/mgC1 |

**Table 50: YIELD CONSTANTS FOR CHEMICAL 1 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| 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 51: YIELD CONSTANTS FOR CHEMICAL 2 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| | | | Y()21: | Yield coefficient for production of C1 from C2, mgC2/mgC1 |
| | 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 C3 from C2, mgC3/mgC2 |
| | 777 | | YBW23 | Water column biodegradation |
| | 779 | | YBS23 | Benthic biodegradation |
| | 847 | | YHOH23 | Alkaline hydrolysis |
| | 849 | | YHN23 | Neutral hydrolysis |
| | 851 | | YHH23 | Acid hydrolysis |

**Table 51: YIELD CONSTANTS FOR CHEMICAL 2 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| | 882 | | YOX23 | Oxidation |
| | 1167 | | YF23 | Photolysis |
| | 1197 | | YE23 | Extra reaction |

**Table 52: YIELD CONSTANTS FOR CHEMICAL 3 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| **C1** | **C2** | **C3** | **Variable** | **Definition** |
| | | | Y()31: | Yield coefficient for production of C1 from C3, mgC1/mgC2 |
| | | 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 C2 from C3, mgC2/mgC3 |
| | | 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 |

## 4.15 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.

**Table 53: DATA GROUP I: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **Number of Time Functions (I10, 70X) - (entered once)** | |
| 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) | T |
| TITLE | name of data group. (70X) | enter "Kinetic Time Functions." |
| **Record 2** | **Time Function Descriptions (A5, 2I5) - (Records 2-3 are input as a group NFUNC times)** | |
| ANAME(ISC) | an optional one to five alphanumeric character descriptive name for the time function I. (A5) | P |
| NOBRK(ISC) | number of breaks used to describe the time function I. (I5) | T |
| ISC | number identifying the time function; these numbers are set by the model developer. (I5) | T |
| **Record 3** | **Time Functions (4(2F10.0)) - (repeated NOBRK(ISC)/4 times, uses as many four VALK(K)-T(K) pairs on 80-space lines as needed to input NOBRK entries)** | |
| VALT(K) | value of time function ISC at time T(K). (F10.0) | T |
| 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) | T |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

### 0.0.9 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.

**Table 54: TIME FUNCTIONS FOR EUTROPHICATION**

| ISC | ANAME | Definition and Units |
|---|---|---|
| 1 | TEMP(1) | Time-variable temperature function 1. TEMP(K) can be either a normalized function or an actual temperature in °C, depending upon the definition of the parameter multiplier TMPSG(ISEG). |
| 2 | TEMP(2) | Time-variable temperature function 2, unitless or °C. |
| 3 | TEMP(3) | Time-variable temperature function 3, unitless or °C. |
| 4 | TEMP(4) | Time-variable temperature function 4, unitless or °C. |
| 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, °C. 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. |

### 0.0.10 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.

**Table 55: TIME FUNCTIONS FOR TOXI4**

| 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 °C, depending upon the definition of the parameter multiplier TEMP(ISEG). |
| 2 | TEMPN(2) | Time variable temperature function 2, unitless or °C. |
| 3 | TEMPN(3) | Time variable temperature 3, unitless or °C. |
| 4 | TEMPN(4) | Time variable temperature 4, unitless or °C. |
| 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 |

**Table 55: TIME FUNCTIONS FOR TOXI4**

| ISC | ANAME | VALT(ISC) |
|---|---|---|
| 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.

## 4.16 Data Group J: Initial Conditions

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

**Table 56: DATA GROUP J: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 1** | **System Information (A40, I5, F5.0, F10.0, 20X) - (Records 1-2 are input as a group NOSYS times)** | |
| CHEML | chemical or system name (A40). | P |
| IFIELD | solids field (3, 4, or 5) that transports this system in its pure or sorbed form (I5). | P |
| DSED | density of system; 0.0 for chemical, 0.5-2.5 for solids, kg/L. (F5.0). | P |
| CMAX | maximum concentration allowed, mg/L. (F10.0) | P |
| TITLE | name of data group. (20X) | enter: "Initial Conditions." |

**Table 56: DATA GROUP J: RECORD FORMATS**

| Record & Variable | Description | Input Type[a] |
|---|---|---|
| **Record 2** | **Initial Conditions (3(A5, 2F10.0)) - (repeated NOSEG/3 times, 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)** | |
| ANAME(K) | an optional one to five alphanumeric character descriptive name or number identifying segment K. (A5) | P |
| C(ISYS,K) | initial concentration in segment K of system ISYS in the appropriate units, mg/L. (F10.0) | P |
| DISSF | dissolved fraction of chemical in segment K. (F10.0) | P |

a. N = Node data, S = Segment Data, T= Time-line Data, and P = Project Data for the Entire Network

### 0.0.11 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.

### 0.0.12 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.