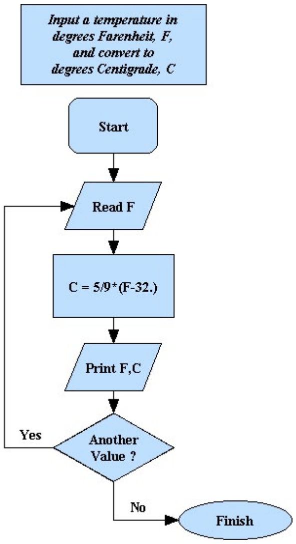
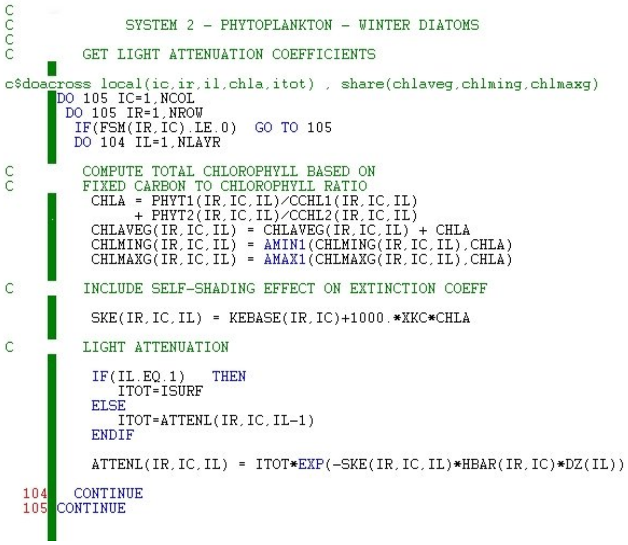
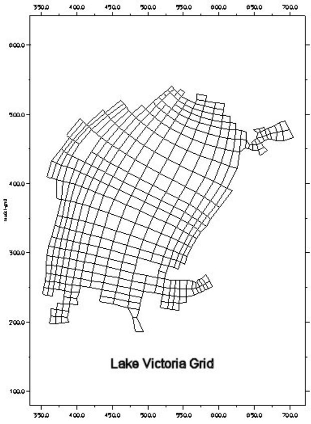
USER'S GUIDE FOR RCA
(Release 3.0)

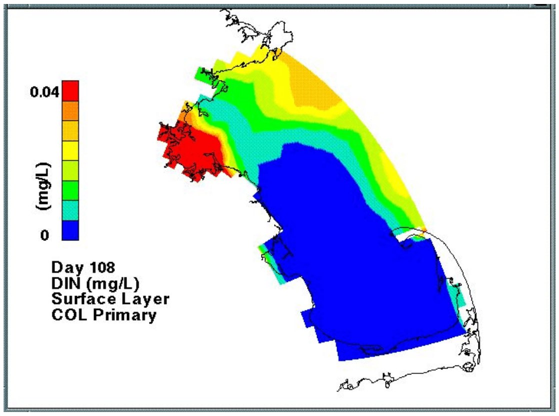
JUNE 2004





```
C
C             SYSTEM 2 - PHYTOPLANKTON - WINTER DIATOMS
C
C        GET LIGHT ATTENUATION COEFFICIENTS

c$doacross local(ic,ir,il,chla,itot) , share(chlaveg,chlming,chlmaxg)
      DO 105 IC=1,NCOL
       DO 105 IR=1,NROW
        IF(FSM(IR,IC).LE.0)  GO TO 105
        DO 104 IL=1,NLAYR

C        COMPUTE TOTAL CHLOROPHYLL BASED ON
C        FIXED CARBON TO CHLOROPHYLL RATIO
          CHLA = PHYT1(IR,IC,IL)/CCHL1(IR,IC,IL)
               + PHYT2(IR,IC,IL)/CCHL2(IR,IC,IL)
          CHLAVEG(IR,IC,IL) = CHLAVEG(IR,IC,IL) + CHLA
          CHLMING(IR,IC,IL) = AMIN1(CHLMING(IR,IC,IL),CHLA)
          CHLMAXG(IR,IC,IL) = AMAX1(CHLMAXG(IR,IC,IL),CHLA)

C        INCLUDE SELF-SHADING EFFECT ON EXTINCTION COEFF

          SKE(IR,IC,IL) = KEBASE(IR,IC)+1000.*XKC*CHLA

C        LIGHT ATTENUATION

          IF(IL.EQ.1)   THEN
             ITOT=ISURF
          ELSE
             ITOT=ATTENL(IR,IC,IL-1)
          ENDIF

          ATTENL(IR,IC,IL) = ITOT*EXP(-SKE(IR,IC,IL)*HBAR(IR,IC)*DZ(IL))

  104   CONTINUE
  105 CONTINUE
```





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PREFACE

The purpose of this manual is to describe the inputs (and their associated formats) required to use the generalized HydroQual water quality model, RCA (an acronym for Row-Column AESOP). The manual also documents the procedure to follow to generate an executable version of the RCA program.

RCA is an extension to the family of generalized water quality models developed by HydroQual (and its predecessor firm Hydroscience). The original member of the family was known as WASP (Water Analysis Simulation Program) and was developed in the early 1970s at Hydroscience. This program was later provided to the U.S. EPA and continues to be supported by the EPA's Center for Water Quality Modeling. The most recent version is WASP6. The second generation of the family is known as AESOP (Advanced Ecological Systems Modeling Program) and was also developed by Hydroscience in the mid- to late-1970s. AESOP provided considerable improvements over the original WASP code including: a more computationally efficient numerical integration scheme (implicit integration); a more flexible computer coding approach for generating variable-configuration versions (i.e., number of systems by number of segments) of the code; addition of system dependent transport; and, in the mid-1980s, a preliminary link to HydroQual's generalized circulation model, ECOM, which was developed by Blumberg and Mellor (1987).

The newest member of the family, RCA (Row-Column AESOP), is meant to provide a WASP/AESOP-compatible computational framework for fine-mesh grids that can be used in conjunction with hydrodynamic applications for large lakes, rivers, and estuarine and coastal systems. RCA is able to directly interface with ECOM and ECOMSED and utilizes the same model grid and geometry and bathymetric information as used by the hydrodynamic model. RCA uses the transport fields that result from the hydrodynamic computation to compute the transport of water quality variables of interest within the study domain. In addition, since computing water quality on the same grid as used by the hydrodynamic model can be computationally expensive, options exist within RCA to take advantage of grid-aggregation programs. These grid-aggregation programs provide the user with a means of aggregating or collapsing the fine-grid hydrodynamic model into a coarser-grid representation suitable for water quality computational purposes.

Since RCA is a descendant of AESOP, much of the input structure and nomenclature is the same as is incorporated in AESOP. Therefore, a user familiar with AESOP should be able to set up a RCA input file without too much difficulty.

The interfacing between RCA and ECOM has been checked extensively (and recognition is extended to Kai-Yuan Yang and Eugenio Gomez-Reyes for their concerted efforts in this task) in this release of RCA. RCA has been demonstrated to exactly reproduce salinity fields computed by the ECOM/ECOMSED model, when run using the same integration procedure (the center-differenced in time and space, leap-frog scheme) as ECOM/ECOMSED. RCA also compares favorably to ECOM/ECOMSED salt computations when run using the upwind or backward difference scheme with Smolarkiewicz correction applied.

As stated above the purpose of this manual is to document the model inputs and input structure required to set up and perform a water quality simulation using RCA. As such the user's guide provides a brief description of the required input fields, the associated units (e.g. m/sec, kg/day, etc.) expected by RCA, and the input options available to the user should more than one type of input for a input group be permitted.

All ideas and critical comments concerning improvements (typos, sections requiring greater clarity in writing and purpose, etc.) which could be made to this document are welcomed by its author and should be directed to the undersigned. Kai-Yuan Yang is also recognized for his valuable contributions in integrating the various "versions" of RCA that have been spawned since RCA Version 2.0 into the new RCA 3.0 documented in this manual. Linda Jensen is also recognized for her patience and perseverance in preparing this Users Guide.

James J. Fitzpatrick

1.0 Introduction

RCA is a Row-Column version of AESOP, HydroQual's general purpose water quality modeling computer code. RCA was developed to directly interface with HydroQual's general circulation model, ECOMSED. As such, it will eliminate the need to use ECOSOP, the hydrodynamic to water quality model interface program that is required to link ECOMSED and AESOP.

Both RCA and AESOP solve general mass balance equations for water quality variables of interest. The principle difference between RCA and AESOP is that RCA obtains it advective and dispersive transport fields from a hydrodynamic model, whereas in AESOP the transport fields are specified by the user, based on kinematic box analysis or via calibration to a conservative tracer variable such as salinity.

A second difference between the two computer codes is that RCA has been written to take advantage of the parallel processing capabilities of CRAY or SGI computer systems and, therefore, should be faster than an equivalent AESOP model with the same number of segments.

1.1 Characteristics of the Model

Generality

RCA (as is AESOP) is a general purpose code developed to be used to evaluate a myriad of water quality problem settings. The user is able, via the development of a FORTRAN subroutine, to tailor RCA to address the specific water quality issues of the water body under investigation. The FORTRAN subroutine (called TUNER) prescribes the biological, chemical and/or physical kinetics or interrelationships between the relevant water quality variables of interest.

Mass Balance

RCA formulates mass balance equations for each model segment for each water quality constituent or state-variable of interest. These mass balance equations include all horizontal, lateral and vertical components of advective flow and dispersive mixing between model segments; physical, chemical and biological transformations between the water quality variables within a model segment; and point, nonpoint, fall-line and atmospheric inputs of the various water quality variables of interest.

Finite Difference

The partial differential equations, which form the water quality model, together with their boundary conditions, are solved using mass conserving finite difference techniques, Equation 1.

$$\frac{dM_i}{dt} = C_i \frac{dV_i}{dt} + V_i \frac{dC_i}{dt} \tag{1a}$$

$$\frac{dV_i}{dt} = \sum Q_{in} - \sum Q_{out} \tag{1b}$$

$$\begin{aligned} \frac{dC_i}{dt} = {} & \sum \frac{Q_{in}}{V_i} \left(\alpha\, C_{up} + (1-\alpha)\, C_i \right) - \sum \frac{Q_{out}}{V_i} \left(\alpha\, C_i + (1-\alpha)\, C_{dwn} \right) \\ & + \sum \frac{R_{ij}}{V_i} \left(C_j - C_i \right) + \frac{W_i}{V_i} \pm k_i\, C_i \end{aligned} \tag{1c}$$

where

M_i = mass of substance in segment i (kg),
C_i = concentration of substance in segment i (mg/L),
V_i = volume of segment i (m^3),
t = time,
Q_{in} = flow(s) entering segment i (m^3/sec),
Q_{out} = flow(s) leaving segment i (m^3/sec),
α = weighting or differencing factor,
= 1 for upwind scheme,
= 0.5 for central differencing scheme,
C_{up} = concentration of substance entering segment i due to Q_{in}, i.e., the concentration in the "upstream" segment (mg/L),
C_{dwn} = concentration of substance in the "downstream" segments associated with Q_{out} (mg/L),
R_{ij} = bulk exchange coefficient between segments i and j (m^3/sec),
C_j = concentration of substance in segment j (mg/L),
W_i = load or source input of substance i (kg/day),
k_i = reaction of substance in segment i (day^{-1}).

Each water quality segment or grid cell is assumed to be completely mixed, i.e., the concentrations of each water quality variable are uniform within the model segment or grid cell. Two finite difference approximations are available for the space derivatives: central difference, which introduces little or no artificial diffusion; and backward or upwind difference, which introduces an artificial diffusion that is proportional to the advective velocity and the grid size, as per Equation 2:

$$E_{num} = \frac{u\Delta x}{2} \tag{2}$$

where

E_{num} is the artificial or numerical diffusion (m^2/sec),
u is the advective velocity (m/sec),

Δx is the grid spacing (m).

Ideally, one would want to utilize central difference approximations in water quality modes, since no artificial diffusion is introduced into the model solution. However, the use of central differences can introduce other "problems" (but not errors) into the solution of the model equations. In particular, the use of central differences does not guarantee positivity, i.e. "negative" concentrations can be computed, although mass is conserved. Nor do central differences resolve step functions or delta functions, as might be introduced by point source inputs or intermittent CSO inputs, in a desirable fashion. The specification of these "abrupt" inputs can result in the generation of "saw-toothed" solutions, i.e. small oscillations about the mean concentration profile, along a spatial gradient, or "in a purely advective system" the apparent propagation of concentration upstream of a pollutant discharge. Again, these characteristics are not "errors" in the solution, but rather undesirable features resulting from the use of central differences in an attempt to eliminate numerical dispersion. While the central difference algorithm is available for use in RCA applications, it is recommended that it not be used because of the aforementioned problems.

As noted above, backward or upwind finite difference approximations to the continuous partial differential mass balance equation are also included as an option in RCA. While upwind differences do maintain positivity and do not generate "saw-toothed" solutions, they do introduce numerical dispersion into the finite difference equations. For certain problems, the magnitude of this numerical dispersion might be sufficient to eliminate or significantly reduce concentration gradients in the vertical or horizontal planes. To partially alleviate this problem, RCA has been coded with an additional user selectable option that permits the use of an upwind corrector scheme, based on Smolarkiewicz's antidiffusive velocity algorithm, which reduces the magnitude of the numerical dispersion in the finite difference solution. While this option can significantly improve the resolution of vertical and horizontal concentration gradients by RCA, it does so at the cost of additional computational overhead (20 to 50 percent increases in run-time).

Solution Options

RCA provides the user with a number of numerical schemes for solving the water quality mass balance equations. In time-variable mode, the user may utilize one of five explicit time-stepping algorithms, all of which require that the time-step (Δt) obey Equation 3:

$$\Delta t \leq \mathrm{Min}\left(\frac{V}{\sum Q + \sum R + kV}\right) \tag{3}$$

where

Δt is the maximum time-step or integration interval (secs),
V is the segment volume (m^3),
$\sum Q$ is the sum of the advective fluxes leaving the segment (m^3/sec),

$\sum R$ is the sum of the dispersive fluxes leaving the segment (m^3/sec),
kV is the loss rate of material due to kinetic reactions (m^3/sec).

The five algorithms include: (1) a centered-in-time Smolarkiewicz-corrected upwind scheme; (2) forward-in-time (first order Euler) with and (3) without Smolarkiewicz correction upwind schemes; (4) and split-timestep with and (5) without Smolarkiewicz correction upwind schemes.

Two modifications have been implemented within RCA to reduce run times for computationally-intensive applications. First, an option to evaluate the kinetic portion of the mass balance equation on a less frequent basis than the transport portion of the equation is evaluated and, second, a split-timestep integration procedure. The first modification assumes that the kinetics or reaction rates of the problem have much lower time constants than do the transport, i.e., the biological or chemical reaction rates on the order of 0.01 to 0.2/day versus equivalent transport rates of 1 to 10/day or greater (equivalent to detention times of 1 to 0.1 days or less). If, for example, a model investigation of eutrophication requires a timestep of 0.01 day (about a quarter hour) to meet the stability criteria of Equation 3, a user might wish to select the option in RCA which permits the kinetic subroutine (TUNER) to be evaluated every 0.10 days, rather the 0.01 day required for the transport. Selecting this option might permit a savings of 20 to 30 percent of the runtime. However, it is recommended that all final calibration runs and all projection runs be performed with the kinetic routine called every transport timestep. This ensures that no "errors" are introduced into the model solution. One way to determine the maximum stepsize for evaluating the kinetic subroutine is to perform a number of simulations, wherein the stepsize for evaluating the kinetics is increased each time and the computational results are compared against a run wherein the kinetic and transport stepsizes are the same, i.e., the base case. The user could then pick a stepsize value for evaluating the kinetics, which minimizes computer runtime, but does not significantly affect the computational results relative to the base case.

The second modification (available in the "in-house" version of RCA), split time-step integration, permits the integration of the "critical detention time" segments using a small timestep to maintain stability for the critical segments, while integrating the remaining (majority) of the water quality segments using a larger (factor of 5 to 10) timestep than is required for the critical segments. One of the options available in RCA is to have RCA step through the entire simulation period (or hydrodynamic transport file) to determine the critical integration timesteps for each averaging period within the hydrodynamic record. This diagnostic analysis provides the absolute "critical" timestep required to maintain stability (as defined by Equation 3) and, in addition the critical timestep for 1, 5, 10, 15 and 20 percent of the computational water quality grid. For example, a water quality grid with 5,000 segments might have the following "average" critical timestep characteristics: an absolute critical timestep of 0.0057 days; 1 percent (50 segments) with a critical timestep of 0.0091 days or less; 5 percent (250 segments) with a critical timestep of 0.012 days or less; 10 percent (500 segments) with a critical timestep of 0.021 days or less; 15 percent (750 segments) with a critical timestep of 0.026 days or less; and 20 percent (1000 segments) with a critical timestep of 0.031 days or less. The user could, then, using the appropriate RCA input options, select a critical or split timestep of 0.005 days and a full timestep of 0.025 days (and possibly further select a kinetic subroutine timestep of 0.10 days). This could result in an overall 50 to 75 percent reduction in total computational time over the base case, where all segments are integrated using a timestep of 0.005 days and a kinetic timestep of 0.005 days. Once again the user is urged to perform a number of runs in order to evaluate the sensitivity of the model solution to the split time-step integration stepsize.

Variable Grid Size and Sigma-Level and Z-Level Coordinates

Since RCA depends upon the hydrodynamic model, ECOMSED, for its model geometry and transport fields, it employs the same variable horizontal grid and vertical (either sigma- or Z-level) coordinate system as does ECOMSED. (For further information on sigma coordinates and the HydroQual general circulation model the user is referred to the ECOMSED Primer.) While the user may run RCA using a sigma-level coordinate system, RCA will still permit the user to specify boundary condition and initial conditon inputs using standard (or fixed depth) levels. RCA then transforms the standard level inputs to the sigma-level grid using linear interpolation.

Flexible Specification of Pollutant Inputs

RCA permits the user to specify pollutant inputs using any or all of four categories: point source (WWTPs/CSOs/SSOs), nonpoint source (urban/agricultural/ watershed runoff), fall-line or riverine sources, and atmospheric source (wetfall/dryfall). Although all pollutant inputs could be organized and input into the model as one loading group, as is done in AESOP, it was thought that permitting these four groupings in RCA would provide the user with greater flexibility in structuring his/her input deck. By splitting the inputs into four groups, the user can perform sensitivity or component analysis much easier by just setting the scale factor for the appropriate group to the desired value rather than be forced to edit the input file and modify a large group of numbers that correspond to the loading group to be analyzed. An example of this would be to reduce all STP and CSO inputs by fifty percent but keep all non-point source, riverine and atmospheric loadings the same. To do this the user would need only to set the scale factor of the point source loading group to 0.5, leaving all other inputs to the model the same.

Flexible Disk Storage of Computational Results

RCA permits the user two types of storage for computational results: (1) domain-wide or "global" dumps of all state-variables at "coarse" time intervals; and/or (2) detailed dumps for selected segments at "fine" time intervals. In the first instance a user could save concentrations for all state-variables over the entire model domain for a period of a year using 10 day intervals. This would permit the user using the HydroQual post-processing tool H4D to generate contour plots or time-variable movies for any plane within the model. When using detailed dumps a user can generate more detailed information concerning model performance by saving secondary variables, such as total extinction coefficients, nutrient limitation terms, etc., as well as the state-variable concentrations for selected segments within the model, at one day intervals. The user could then generate detailed time-series plots using HydroQual post-processing tool GDP. (Note: the information contained in the detailed dumps is determined in the TUNER subroutine via a series of CALLs to the subroute RCAWBUF. A more complete description of the structure of the RCA output files is contained in Appendix D.)

Enhancements to RCA Version 3.0

A number of enhancements have been made between this release of RCA (Version 3.0) and previous versions of the code. These include:

- implementation of an integer "clock" to control the overall numerical simulation and the updating of hydrodynamic, load, and boundary condition inputs,
- a revised input structure for specifying point, nonpoint, and fall line loads that includes provision for specifying a load identification table,
- implementation of piece-wise linear interpolation of load inputs,
- greater checking for input errors, and
- use of comment or header records for input records to facilitate editing or modification of required input information.

In previous versions of RCA a real-time clock (in days) was used by RCA to keep track of the simulation time and coordinate with updating of time-variable models inputs such as generated by the hydrodynamic model ECOMSED or loadings and/or boundary conditions. Unfortunately, the use of REAL variables can result in numerical round-off errors after repeated addition of fractions. This can result in synchronization errors when updating the hydrodynamic model inputs. Therefore, RCA has been modified to use INTEGER variables to specify the numerical time-step for integration and to keep track of the simulation time. These internal variables will operate in units of seconds.

RCA has also been modified so that pollutant loads can be specified using piece-wise linear interpolation rather than just step function changes. As an example suppose a user specifies the following time-series input for a pollutant load:

value	time	value	time	value	time
10.0	0.0	20.0	50.0	40.0	100.

If the user selected the step-function option, the value of the pollutant load at time = 25 would be 10.0. If, however, the user selected piece-wise linear interpolation the value at time = 25 would be 15.

Version 3.0 of RCA has also been improved to provide greater checking of model inputs. For example, RCA will check to make sure that the model segment to which a pollutant load is assigned is a valid water cell.

Finally, for normal Ascii (or card-image) files, RCA has been modified to include a "comment" or "header" record to be read before every major input record. Although the user may leave these records "blank" without any consequence, use of these comment records to list or describe the input data to follow may facilitate subsequent editing or modification of the input data required to run the model. It should be noted, however, that comment or header records SHOULD NOT be included in binary files.

1.2 Getting Started

Hydrodynamic Model Files

In order to begin, the user will, of course, need a hydrodynamic model. The hydrodynamic model code, ECOMSED, generates three output files (four, if the user chooses to save only the water cells of the model grid) which are required by RCA. These files are named, "gcm_geom," which contains information concerning model geometry, "gcm_tran" which contains the advective and dispersive transport fields, and "gcm_gdiff" which contains information relating to the locations and time-variable discharge volumes associated with any diffusers or outfalls included in the hydrodynamic model (and "wet_grid," which contains the locations of the water cells in the model domain, if the "water cells only" option is chosen). The user will need to move, copy, or link the "gcm_geom" and "wet_grid", if appropriate, files to the directory in which the water quality model and the executable version of RCA are to reside. The "gcm_tran" file(s) and "gcm_gdiff" file(s), however, need not be moved, copied, or linked. They can remain in a separate directory, file folder, or disk drive.

TUNER Subroutine

Next the user will be required to supply a FORTRAN subroutine, which contains the state-equations or kinetics for the water quality problem of interest. The subroutine should be called "TUNER" (as in SUBROUTINE TUNER) but may be maintained on the system using any name that the user desires (for example, lisem2.f). An example TUNER, written for a one-system conservative tracer, which can also be used to calculate residence time of a waterbody (and which can be easily expanded to three-systems) is presented in Table 1. Appendices A and B provide descriptions of more complex TUNERS; one that is HydroQual's current implementation of eutrophication kinetics and one that is HydroQual's current implementation of coliform kinetics and that are provided as part of the public domain release of RCA. Appendix C provides more detail on the residence time subroutine presented in Table 1.

TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER

```
C
C***********************************************************************
C
      SUBROUTINE   TUNER
C
C***********************************************************************
C
C          RESIDENCE TIME MODEL - COMPUTE RESIDENCE TIME OF A SEGMENT(s)
C          -------------------------------------------------------------
C               (Note: current version is set up for 1 system, but may
C                  be readily expanded to 2 or 3 systems by uncommenting
C                  the appropriate FORTRAN statements in the code)
C
C***********************************************************************
C
C     SYSTEMS                                                      UNITS
C     -------                                                      -----
C        1 - DYE1  - CONCENTRATION OF DYE                           MG/L
C        2 - DYE2  - CONCENTRATION OF DYE                           MG/L
C        3 - DYE3  - CONCENTRATION OF DYE                           MG/L
C
C***********************************************************************
C
C     CONSTANTS
C     ---------
C
C   NO   NAME      DESCRIPTION                                     UNITS
C   --   --------  ----------------------------------------------- -----
C    1   DYEDIS1   DYE DISTRIBUTION OPTION
C                  = 0, ASSIGN INITIAL DYE CONCENTRATIONS UNIFORMLY
C                       THROUGHOUT THE WATER COLUMN (I.E., TOP TO
C                       BOTTOM) USING PARAM2D(1)
C                       PARAM2D(2) WILL BE USED TO SPECIFY THE DOMAIN
C                       OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED
C                  = 1, INITIAL DYE CONCENTRATIONS WILL BE SPECIFIED
C                       ON A SEGMENT BY SEGMENT BASIS USING PARAM3D(1)
C                       PARAM3D(2) WILL BE USED TO SPECIFY THE DOMAIN
C                       OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED
C    2   TIMEDYE1  TIME TO RELEASE DYE 1
C    3   DECAY1    DECAY RATE FOR DYE 1                             /DAY
C    4   DYEDIS2   DYE DISTRIBUTION OPTION
C                  = 0, ASSIGN INITIAL DYE CONCENTRATIONS UNIFORMLY
C                       THROUGHOUT THE WATER COLUMN (I.E., TOP TO
C                       BOTTOM) USING PARAM2D(3)
C                       PARAM2D(4) WILL BE USED TO SPECIFY THE DOMAIN
C                       OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED
C                  = 1, INITIAL DYE CONCENTRATIONS WILL BE SPECIFIED
C                       ON A SEGMENT BY SEGMENT BASIS USING PARAM3D(3)
C                       PARAM3D(4) WILL BE USED TO SPECIFY THE DOMAIN
C                       OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED
C    5   TIMEDYE2  TIME TO RELEASE DYE 2
C    6   DECAY2    DECAY RATE FOR DYE 2                             /DAY
C    7   DYEDIS3   DYE DISTRIBUTION OPTION
C                  = 0, ASSIGN INITIAL DYE CONCENTRATIONS UNIFORMLY
C                       THROUGHOUT THE WATER COLUMN (I.E., TOP TO
C                       BOTTOM) USING PARAM2D(5)
C                       PARAM2D(6) WILL BE USED TO SPECIFY THE DOMAIN
C                       OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED
C                  = 1, INITIAL DYE CONCENTRATIONS WILL BE SPECIFIED
C                       ON A SEGMENT BY SEGMENT BASIS USING PARAM3D(5)
C                       PARAM3D(6) WILL BE USED TO SPECIFY THE DOMAIN
C                       OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED
C    8   TIMEDYE3  TIME TO RELEASE DYE 3
C    9   DECAY3    DECAY RATE FOR DYE 3                             /DAY
C
C***********************************************************************
C
C     2-D PARAMETERS
C     --------------
C
C       NO  NAME          DESCRIPTION                              UNITS
C      ---  --------  -------------------------------------------  -----
C        1  DYE1IC2   INITIAL CONDITIONS FOR DYE1                   MG/L
C        2  DOMAIN1   DOMAIN FOR DETERMINING RESIDENCE TIME 1
C        3  DYE2IC2   INITIAL CONDITIONS FOR DYE2                   MG/L
C        4  DOMAIN2   DOMAIN FOR DETERMINING RESIDENCE TIME 2
C        5  DYE3IC2   INITIAL CONDITIONS FOR DYE3                   MG/L
C        6  DOMAIN3   DOMAIN FOR DETERMINING RESIDENCE TIME 3
C
C***********************************************************************
C
```

TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER (Cont.)

```
C     3-D PARAMETERS
C     --------------
C
C       NO  NAME           DESCRIPTION                              UNITS
C      ---  --------  ------------------------------------------   -----
C        1  DYE1IC3   INITIAL CONDITIONS FOR DYE1                      MG/L
C        2  DOMAIN1   DOMAIN FOR DETERMINING RESIDENCE TIME 1
C        3  DYE2IC3   INITIAL CONDITIONS FOR DYE2                      MG/L
C        4  DOMAIN2   DOMAIN FOR DETERMINING RESIDENCE TIME 2
C        5  DYE3IC3   INITIAL CONDITIONS FOR DYE3                      MG/L
C        6  DOMAIN3   DOMAIN FOR DETERMINING RESIDENCE TIME 3
C
C***********************************************************************
C
C     TIME-VARIABLE FUNCTIONS
C     -----------------------
C           NONE
C
C***********************************************************************
C
      SAVE

      INCLUDE 'RCACM'
      CHARACTER   GDNAMES(NOSYS)*8,DDNAMES(5,NOSYS)*8

C        STATE-VARIABLES
      REAL
     .      DYE1(NX,NY,NZ)
CC   .    , DYE2(NX,NY,NZ)
CC   .    , DYE3(NX,NY,NZ)
      EQUIVALENCE
     .      (CARAY(1,1,1,1),DYE1(1,1,1))
CC   .    , (CARAY(1,1,1,2),DYE2(1,1,1))
CC   .    , (CARAY(1,1,1,3),DYE3(1,1,1))
      REAL
     .      DYE_DDA(NX,NY,NZ,NOSYS)
     .    , DYE_DMIN(NX,NY,NZ,NOSYS)
     .    , DYE_DMAX(NX,NY,NZ,NOSYS)
     .    , DYE_GDA(NX,NY,NZ,NOSYS)
     .    , DYE1_GDA(NX,NY,NZ)
C    .    , DYE2_GDA(NX,NY,NZ)
C    .    , DYE3_GDA(NX,NY,NZ)
      EQUIVALENCE
     .      (DYE_GDA(1,1,1,1),DYE1_GDA(1,1,1))
C    .    , (DYE_GDA(1,1,1,2),DYE2_GDA(1,1,1))
C    .    , (DYE_GDA(1,1,1,3),DYE3_GDA(1,1,1))

C        CONSTANTS
      EQUIVALENCE
     .   (CONST(1),DYEDIS1)  , (CONST(2),TIMEDYE1) , (CONST(3),DECAY1) ,
     .   (CONST(4),DYEDIS2)  , (CONST(5),TIMEDYE2) , (CONST(6),DECAY2) ,
     .   (CONST(7),DYEDIS3)  , (CONST(8),TIMEDYE3) , (CONST(9),DECAY3)

      REAL*8   TOTMASIC(NOSYS),TOTMASREG(NOSYS),TOTMASALL(NOSYS)

      INTEGER*2  SYSGDP(40)
C        INITIAL -SYSBY- SETTINGS
      DATA  SYSGDP/40*1/

C        PROVIDE INITIALIZATION, IF FIRST TIME THROUGH -FABLE-
      IF(INITB.EQ.1)   GO TO 50
C        SET-UP AND WRITE INFORMATION NEEDED BY GDP
        GDNAMES( 1) = 'DYE1'
C       GDNAMES( 2) = 'DYE2'
C       GDNAMES( 3) = 'DYE3'
      DO ISYS=1,NOSYS
         SYSGDP(ISYS) = SYSBY(ISYS)
      ENDDO
      REWIND(10)
      WRITE(10)   NX,NY,NZ,NOSYS,NOSYS
      WRITE(10)   GDNAMES
      WRITE(10)   SYSGDP
      WRITE(10)   FSM
C        WRITE DDNAMES TO RCAF12
C          (NOTE: IF SYSTEM 2 AND/OR 3 ACTIVATED ADD APPROPRIATE DDNAMES)
      IF(IDDOPT.EQ.0) THEN
       DDNAMES(1,1)='    DYE1'
       DDNAMES(1,2)='   DUMMY'
       DDNAMES(1,3)='IC MASS1'
       DDNAMES(1,4)='REGNMAS1'
       DDNAMES(1,5)='DOMNMAS1'
      ELSE
```

TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER (Cont.)

```
       DDNAMES(1,1)='AVE DYE1'
       DDNAMES(1,2)='MAX DYE1'
       DDNAMES(1,3)='IC MASS1'
       DDNAMES(1,4)='REGNMAS1'
       DDNAMES(1,5)='DOMNMAS1'
      ENDIF
      WRITE(12)  DDNAMES

C        SET INITIAL CONDITIONS
      DO 30 ISYS=1,NOSYS
       IF(CONST(3*(ISYS-1)+1).EQ.0 .AND. CONST(3*(ISYS-1)+2).EQ.0.) THEN
         DO 10 IZ=1,NZ
          DO 10 IY=1,NY
           DO 10 IX=1,NX
            IF(FSM(IX,IY).EQ.1.)
     .            CARAY(IX,IY,IZ,ISYS) = PARAM2D(IX,IY,2*(ISYS-1)+1)
   10    CONTINUE
C        RESET CONSTANT SO DYE IS NOT PUT INTO SYSTEM AGAIN
         CONST(3*(ISYS-1)+2)=9.99E+9
       ELSEIF(CONST(3*(ISYS-1)+1).EQ.1 .AND. CONST(3*(ISYS-1)+2).EQ.0.)
     .  THEN
         DO 20 IZ=1,NZ
          DO 20 IY=1,NY
           DO 20 IX=1,NX
            IF(FSM(IX,IY).EQ.1.)
     .            CARAY(IX,IY,IZ,ISYS) = PARAM3D(IX,IY,IZ,2*(ISYS-1)+1)
   20    CONTINUE
         CONST(3*(ISYS-1)+2)=9.99E+9
       ENDIF
   30 CONTINUE
      CALL RCA09
      IREC=IREC-1

C        INITIALIZE ARRAY FOR GLOBAL DUMP AVERAGING, IF REQUIRED
      IF(IGDOPT.EQ.1)  THEN
       DO 40 ISYS=1,NOSYS
        DO 35 IZ=1,NZ
         DO 35 IY=1,NY
          DO 35 IX=1,NX
            DYE_GDA(IX,IY,IZ,ISYS) = 0.
            DYE_DDA(IX,IY,IZ,ISYS) = 0.
            DYE_DMIN(IX,IY,IZ,ISYS) = 1000.
            DYE_DMAX(IX,IY,IZ,ISYS) = -1000.
   35   CONTINUE
   40  CONTINUE
       IAVGGDCNTR = 0
       IAVGDDCNTR = 0
       IAVGPPCNTR = 0
      ENDIF
      DUMMY=0.0

   50 CONTINUE

C        CHECK IF TIME TO LOAD ANOTHER DYE
      DO 100 ISYS=1,NOSYS
       IF(CONST(3*(ISYS-1)+1).EQ.0 .AND. TIME.GT.CONST(3*(ISYS-1)+2))
     .  THEN
         WRITE(OUT,1200)  ISYS,TIME
 1200    FORMAT(//10X,'LOADING TRACER #',I2,' AT TIME',F8.2)
         DO 70 IZ=1,NZ
          DO 70 IY=1,NY
           DO 70 IX=1,NX
            CARAY(IX,IY,IZ,ISYS) = PARAM2D(IX,IY,2*(ISYS-1)+1)
   70    CONTINUE
         CONST(3*(ISYS-1)+2)=9.99E+9
         CALL RCA09
         IREC=IREC-1
       ELSEIF(CONST(3*(ISYS-1)+1).EQ.1.AND.TIME.GT.CONST(3*(ISYS-1)+2))
     .  THEN
         WRITE(OUT,1200)  ISYS,TIME
         DO 80 IZ=1,NZ
          DO 80 IY=1,NY
           DO 80 IX=1,NX
            CARAY(IX,IY,IZ,ISYS) = PARAM3D(IX,IY,IZ,2*(ISYS-1)+1)
   80    CONTINUE
         CONST(3*(ISYS-1)+2)=9.99E+9
         CALL RCA09
         IREC=IREC-1
       ENDIF
  100 CONTINUE

C        LOOP FOR DETAILED DUMP AVERAGING, IF REQUIRED
```

TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER (Cont.)

```
      IF(IDDOPT.EQ.1)  THEN
       DO 125 ISYS=1,NOSYS
        DO 120 IZ=1,NZ
         DO 120 IY=1,NY
          DO 120 IX=1,NX
            DYE_DDA(IX,IY,IZ,ISYS) = DYE_DDA(IX,IY,IZ,ISYS)
     .          + CARAY(IX,IY,IZ,ISYS)
            DYE_DMIN(IX,IY,IZ,ISYS) =
     .          AMIN1(DYE_DMIN(IX,IY,IZ,ISYS),CARAY(IX,IY,IZ,ISYS))
            DYE_DMAX(IX,IY,IZ,ISYS) =
     .          AMAX1(DYE_DMAX(IX,IY,IZ,ISYS),CARAY(IX,IY,IZ,ISYS))
  120   CONTINUE
  125  CONTINUE
        IAVGDDCNTR = IAVGDDCNTR + 1
      ENDIF

C        SYSTEM 1(-3) - DYE1(-3)
      DO 150 ISYS=1,NOSYS
       TOTMASIC(ISYS)=0.
       TOTMASREG(ISYS)=0.
       TOTMASALL(ISYS)=0.
       DO 135 IZ=1,NZ
        DO 135 IY=1,NY
         DO 135 IX=1,NX
          IF(FSM(IX,IY).NE.1.)  GO TO 135
          CDARAY(IX,IY,IZ,ISYS) = -CONST(3*ISYS)*CARAY(IX,IY,IZ,ISYS)
          IF(IDISK.NE.0) THEN
           IF(CONST(3*(ISYS-1)+1).EQ.0.) THEN
            IF(PARAM2D(IX,IY,2*(ISYS-1)+1).GT.0.)  TOTMASIC(ISYS) =
     .           TOTMASIC(ISYS) + BVOL(IX,IY,IZ)*CARAY(IX,IY,IZ,ISYS)
            IF(PARAM2D(IX,IY,2*ISYS).GT.0.)  TOTMASREG(ISYS) =
     .           TOTMASREG(ISYS) + BVOL(IX,IY,IZ)*CARAY(IX,IY,IZ,ISYS)
           ELSE
            IF(PARAM3D(IX,IY,IZ,2*(ISYS-1)+1).GT.0.)  TOTMASIC(ISYS) =
     .           TOTMASIC(ISYS) + BVOL(IX,IY,IZ)*CARAY(IX,IY,IZ,ISYS)
            IF(PARAM3D(IX,IY,IZ,2*ISYS).GT.0.)  TOTMASREG(ISYS) =
     .           TOTMASREG(ISYS) + BVOL(IX,IY,IZ)*CARAY(IX,IY,IZ,ISYS)
           ENDIF
           TOTMASALL(ISYS) =
     .           TOTMASALL(ISYS) + BVOL(IX,IY,IZ)*CARAY(IX,IY,IZ,ISYS)
          ENDIF
  135  CONTINUE
       IF(IDISK.EQ.2 .OR. IDISK.EQ.3)  THEN
        DO 145 IDMP=1,NDMPS
         IX = IFDMPS(IDMP,1)
         IY = IFDMPS(IDMP,2)
         IZ = IFDMPS(IDMP,3)
         IF(IDDOPT.EQ.0)  THEN
           CALL RCAWBUF(ISYS,CARAY(IX,IY,IZ,ISYS),dummy
     .         ,SNGL(TOTMASIC(ISYS)),SNGL(TOTMASREG(ISYS))
     .         ,SNGL(TOTMASALL(ISYS)))
         ELSE
           CALL RCAWBUF(ISYS,CARAY(IX,IY,IZ,ISYS)/IAVGDDCNTR
     .         ,DYE_DMAX(IX,IY,IZ,ISYS)
     .         ,SNGL(TOTMASIC(ISYS)),SNGL(TOTMASREG(ISYS))
     .         ,SNGL(TOTMASALL(ISYS)))
         ENDIF
  145   CONTINUE
       ENDIF
  150 CONTINUE

C        CONVERT TO MASS UNITS
c$doacross local(iz,iy,ix,isys)
       DO 200 ISYS=1,NOSYS
        DO 200 IZ=1,NZ
         DO 200 IY=1,NY
          DO 200 IX=1,NX
          CDARAY(IX,IY,IZ,ISYS) = BVOL(IX,IY,IZ)*CDARAY(IX,IY,IZ,ISYS)
  200  CONTINUE

      IF(IDISK.EQ.2 .OR. IDISK.EQ.3)  THEN
C        CLOSE BUFFER AND WRITE TO DISK
       CALL RCAWRIT

       DO ISYS=1,NOSYS
        WRITE(OUT,2500)   TOTMASIC(ISYS)/1000.,TOTMASREG(ISYS)/1000.
     .                   ,TOTMASALL(ISYS)/1000.
 2500   FORMAT(
     .     /10X,'INITIAL CONDITION REGIONAL TOTAL MASS =',E13.5,' KG'
     .     /10X,'REGIONAL TOTAL MASS =',E13.5,' KG'/
     .     /10X,'DOMAIN TOTAL MASS =',E13.5,' KG'/)
       ENDDO
```

TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER (Cont.)

```
C        RE-INITIALIZE ARRAY FOR DETAILED DUMP AVERAGING, IF REQUIRED
       IF(IDDOPT.EQ.1)  THEN
        DO 215 ISYS=1,NOSYS
         DO 210 IZ=1,NZ
          DO 210 IY=1,NY
           DO 210 IX=1,NX
             DYE_DDA(IX,IY,IZ,ISYS) = 0.
             DYE_DMIN(IX,IY,IZ,ISYS) = 1000.
             DYE_DMAX(IX,IY,IZ,ISYS) = -1000.
  210    CONTINUE
  215   CONTINUE
        IAVGDDCNTR = 0
       ENDIF
      ENDIF
C        PERFORM GLOBAL DUMP AVERAGING, IF REQUIRED
      IF(IGDOPT.EQ.1)  THEN
       DO 225 ISYS=1,NOSYS
        DO 220 IZ=1,NZ
         DO 220 IY=1,NY
          DO 220 IX=1,NX
            DYE_GDA(IX,IY,IZ,ISYS) = DYE_GDA(IX,IY,IZ,ISYS)
     .                             + CARAY(IX,IY,IZ,ISYS)
  220   CONTINUE
  225  CONTINUE
      ENDIF
      IAVGGDCNTR = IAVGGDCNTR + 1

C         CHECK IF TIME TO DUMP TO DISK
      IF(IDISK.EQ.0)   RETURN
C        GLOBAL DUMPS
      IF(IDISK.EQ.1 .OR. IDISK.EQ.3)  THEN
       IF(IGDOPT.EQ.0)  THEN
         WRITE(10)   TIME
         WRITE(11)   DYE1
C        WRITE(11)  DYE2
C        WRITE(11)  DYE3
       ELSE
         DO 365 ISYS=1,NOSYS
          DO 360 IZ=1,NZ
           DO 360 IY=1,NY
            DO 360 IX=1,NX
             DYE_GDA(IX,IY,IZ,ISYS) = DYE_GDA(IX,IY,IZ,ISYS)/
     .                                           FLOAT(IAVGGDCNTR)
  360     CONTINUE
  365    CONTINUE
         WRITE(10)   TIME - FLOAT(IPRNTGSECS)/86400./2.
         WRITE(11)   DYE1_GDA
C        WRITE(11)   DYE2_GDA
C        WRITE(11)   DYE3_GDA
       ENDIF
       IF(IGDOPT.EQ.1)  THEN
        DO 385 ISYS=1,NOSYS
         DO 380 IZ=1,NZ
          DO 380 IY=1,NY
           DO 380 IX=1,NX
            DYE_GDA(IX,IY,IZ,ISYS) = 0.
  380    CONTINUE
  385   CONTINUE
       ENDIF
       IAVGGDCNTR = 0
       IAVGPPCNTR = 0
      ENDIF

C        INITIAL CONDITION FILE
      REWIND 15
      WRITE(15)  CARAY

      RETURN

  900 WRITE(OUT,9990)
 9990 FORMAT(///5X,'INPUT ERROR WHILE READING IGDOPT,IDDOPT'//)
      CALL EXIT
      END
```

Generating a RCA Executable using "makerca3"

In order to use RCA, the user should copy the RCA source code and makerca3 script from App_Server\Install\RCA to his/her working directory. The user would then execute the "makerca3" script from his/her working directory. This script has options for copying the RCA source code to the working directory, editing various files, compiling the RCA code and building an executable version of RCA. After copying the files, the first task is to edit the "RCACM" file to set the appropriate parameters. These are at the top of the RCACM file in the first PARAMETER statement. The following is a list of variables to be set with a brief description of each:

Variable	Definition
nx	number of grid cells in the x-axis of the model
ny	number of grid cells in the y-axis of in the model
nz	number of grid cells or layers in the vertical plane of the model
nosys	number of systems or water quality state-variables

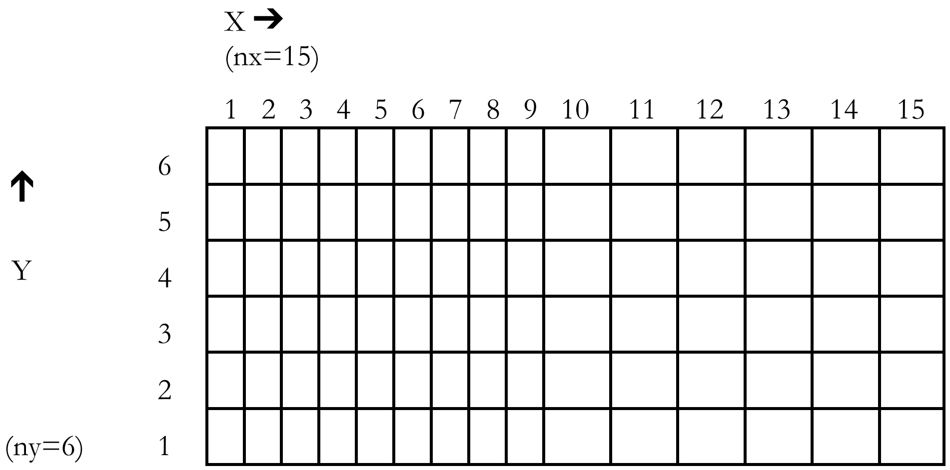
The first few lines of RCACM are listed below:

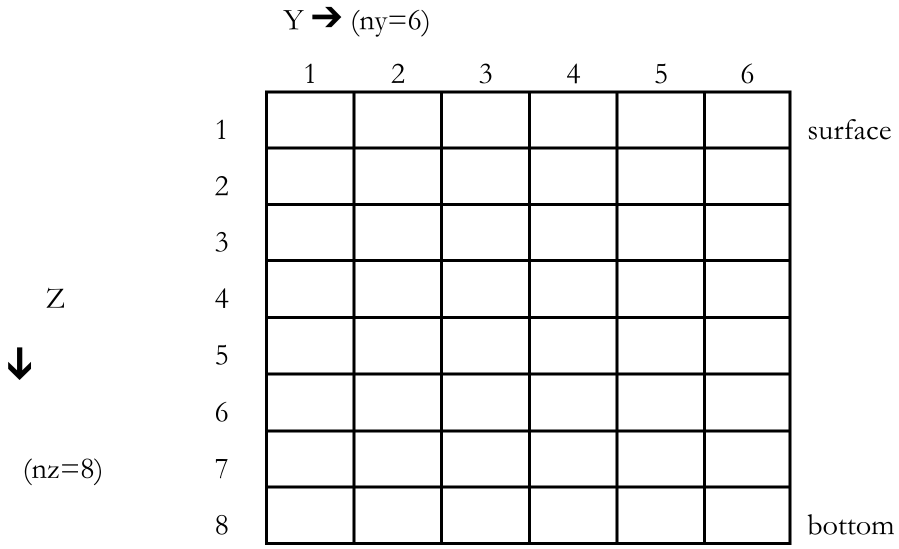
```
C
C    CONFIGURATION, REAL, INTEGER, AND COMMON CARDS FOR RCA
C                                        Version 3.0

     PARAMETER  (NX=nx,NY=ny,NZ=nz,NOSYS=nosys)
     PARAMETER  (NPARM2D=10,NPARM3D=6,NBC=750,NWK=750)
     PARAMETER  (MXCONS=250,MXFUNC=20,MXFUNCT=400)
     PARAMETER (MXHYDFILES=36,NHYD=15000,NSL=100,NSLC=100)
     PARAMETER  (MXSEGSPLT=(NX*NY*NZ)/5)
```

The user would then modify "nx, ny, nz" as per the dimensions required for the model being developed.

An example grid is presented below in order to assist the user in understanding the definitions of nx, ny and nz.





The above "hydrodynamic/water quality grid" has 15 cells in the x-direction, 6 cells in the y-direction and 8 vertical layers.

After editing RCACM, the user should copy the appropriate TUNER.f kinetic subroutine to the CODE directory and compile and build an executable version of RCA using either of the following commands:

> **df /exe:rca_ver3 /convert:BIG_ENDIAN *.f** for a WINDOWS version of RCA -or- **makerca** for a LINUX (UNIX) version of RCA.

1.3 RCA File Structure

During the course of execution RCA requires a number of input files and generates a number of output files. These are briefly described in Table 2. Further details concerning these files will be provided in the following section.

TABLE 2. RCA FILE STRUCTURE

A. USER CREATED INPUT FILES

	NAME	TYPE	CONTENTS
1.	stdin	ASCII	basic input required to run the water quality model
2.	gcm_geom	BINARY	geometry as supplied from the ECOMSED hydrodynamic model
3.	wet_grid	BINARY	row, column (I,J) locations of the water segments in the hydrodynamic model
4.	hydfilna	BINARY	transport terms as supplied from the hydrodynamic model (this is the ECOMSED gcm_tran file)
5.	dffilna	BINARY	diffuser (or outfall) locations and discharge values as supplied from the hydrodynamic model
6	bcfilna	ASCII/binary	boundary condition concentrations for each system
7	psfilna	ASCII/binary	point source loads for each system
8	npsfilna	ASCII/binary	nonpoint source loads for each system
9	flfilna	ASCII/binary	fall-line loads for each system
10	atmfilna	ASCII/binary	atmospheric loads for each system
11	pcfilna	ASCII/binary	model parameters, constants and time-functions as required by the TUNER kinetic subroutine
12	icfilna	ASCII/binary	initial conditions for each system
13	sedfilna	ASCII	input required for applications involving sediment flux models

B. MODEL GENERATED OUTPUT FILES

	NAME	TYPE	CONTENTS
1.	stdout	ASCII	standard output containing all the input information and computed values as selected by the user
2.	RCAF10	BINARY	the system bypass options and times at which the grid-wide dumps were generated
3.	RCAF11	BINARY	a time-history of the grid-wide or global dumps for all state-variables
4.	RCAF12	BINARY	system bypass options, dump variable names and times at which the detailed dumps were generated (for selected segments)
5.	RCAF13	BINARY	a more-detailed time-history dump for selected segments and selected parameters
6.	RCAFIC	BINARY	concentration profiles to be used for multi-year, multi-month, etc. running (provides a "hot start" capability)

TABLE 2. RCA FILE STRUCTURE, Continued

7.	RCAF14	BINARY	the concentrations and fluxes computed by the sediment nutrient flux subroutine, if invoked by the user
8.	RCAFICSED	BINARY	concentration profiles for the sediment for multi-year running (provides a "hot start" capability), if the sediment nutrient flux subroutine is invoked by the user
9.	RCAFMB	BINARY	a time history of mass balance and flux balance terms for the water column
10.	RCAFMBSED	BINARY	a time history of mass balance and flux balance terms for the sediment nutrient flux subroutine

Appendix D provides greater detail as to the "structure" of the RCA output files.

2.0 RCA Model Input Data Description

The inputs required by RCA have been organized into a number of Input Groups and in turn into a number of input files. Table 3 presents the major input groups and associated files (there is a main input file and a number of associated input files):

TABLE 3. LISTING OF MAJOR INPUTS TO RCA BY GROUP

Input Group	File	Description
A	stdin	model descriptor information
B	stdin	print control and integration history
C	stdin	hydrodynamic time breaks and scale factors
D	stdin	names of data files to be used for the input of: boundary conditions; point source loads; nonpoint source loads; fall-line loads; atmospheric loads; parameters, constants and time functions; and initial conditions
E	stdin	stability and accuracy criteria
F	stdin	end of simulation dumps
G	bcfilna	boundary conditions
H	psfilna	point source loads
I	npsfilna	nonpoint source loads
J	flfilna	fall-line loads
K	atmfilna	atmospheric loads
L	pcfilna	parameters, constants and time functions
M	icfilna	initial conditions

GROUP A: MODEL DESCRIPTORS
(STDIN)

One of the major changes in the input structure of RCA input files between Version 2 and Version 3 of the model code is that now RCA requires a comment or title record to be placed before all input records. If the user should so choose, he or she may use the comment line to indicate the variables to be read on the following record. See below for an example.

Inputs required for this group include:

1. linked run option, model listing options, and model execution options
2. model title and run description
3. water quality state-variable names
4. system by-pass options

A1. Linked Run Option, Model Listing Options and Model Execution Options

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60	70	80
CYCLE	LIST1	LIST2	LIST3	LIST4	LIST5	IDIAGDT	INPCHCK

FORMAT(10I10)

CYCLE = linked run option (permits the user to link sequential or multiple year runs together)
= 0, model grid initial conditions are read from the icfilna input file (this is equivalent to a cold-start)
= 1, model grid initial conditions are read from the RCAFIC file, which has been generated by a previous execution of RCA (this is equivalent to a hot-start)
LIST1 = geometry (segment volumes) and transport (flow and dispersion) list option
LIST2 = boundary conditions list option
LIST3 = loadings list option
LIST4 = parameters, constants and time functions list option
LIST5 = initial conditions list option
LIST# = 0, do not list input

= 1, list input
IDIAGDT = execution option
= 0, perform RCA model run
= 1, just run through input deck to determine critical integration timesteps
INPCHCK = input checker option
= 0, perform RCA model run
= 1, just read through input deck to check for input errors

CYCLE should always be equal to 0 for a user's first run and then may be optionally set equal to 1, if the user is performing multi-year (multi-month, etc.) runs using multiple hydrodynamic transport files (gcm_tran). In order to reduce disk storage utilization, it is recommended that the user set LIST# equal to 0 unless performing verification of model inputs.

IDIAGDT can be set equal to 1 on the initial model run in order to determine the critical detention time (and, therefore, maximum timestep size for explicit integration) of the model. Should the user select the split-timestep integration algorithm, setting IDIAGDT will provide useful information for setting both critical and regular timestep sizes. Subsequently, the user would set IDIAGDT to 0 in order to perform full model simulations.

The user should set INPCHCK = 1 the first time running a new input deck to permit RCA to identify any input errors. After an input deck is read without errors, the user can set INPCHCK = 0 and proceed to perform a model simulation.

An example of the use of the "Comment" record and actual input record follows:

```
CYCLE  LIST1  LIST2  LIST3  LIST4  LIST5  IDIAGDT  INPCHCK
    0      0      1      0      0      0        0        1
```

A2. <u>Model Title and Run Description</u>

80
TITLE

FORMAT (A80)

TITLE = user specified title or run description

The user may specify as many lines as desired for the title and/or run description. This input is terminated when RCA encounters a record with "END" or "end" in columns 1-3. For example:

LISS 3.0 Long Island Sound Study - 3-D Version
Uses NOAA Hydrodynamic Files Received 12/04/90

Algal Growth Rates = 2.0 and 0.9 /day   Low Grazing Pressure
Recycle Rates = 0.05 /day   Algal settling is a function of nutrient status
Base settling rate = 0.5 m/day - nutrient depleted settling rate = 0.5 m/day
END

A3. State-Variable Names

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

8	16	24	80
SYNAME(1)	SYNAME(2)	SYNAME(3) - - -	SYNAME(NOSYS)

FORMAT(10A8)

SYNAME(ISYS) = user specified header to describe system ISYS (NOSYS is the total number of systems or state-variables in the water quality model)

Note: Although these system names are not used explicitly in RCA, they will be used when printing input data associated with loads, boundary conditions, and initial conditions. The order of the system names is determined by the user's kinetic subroutine (TUNER).

A4. System Bypass Options

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

2	4	6	80
SYSBY(1)	SYSBY(2)	SYSBY(3) - - -	SYSBY(NOSYS)

FORMAT(40I2)

SYSBY(ISYS) = system bypass option for system ISYS
= 0, include this system in the model computation

= 1, bypass this system in the model computation

The system bypass option permits the user to include or exclude water quality variables from the model computation without performing major revisions to the user supplied inputs. The user should, however, make sure that the TUNER kinetic subroutine is written in such a way as to permit the by-passing or exclusion of the selected state-variables.

GROUP B: PRINT CONTROL AND INTEGRATION CONTROL INFORMATION (STDIN)

Inputs required for this group include:

1. integration solution options,
2. time-warp scale factor and start of simulation time,
3. number of integration step-sizes,
4. integration step-size history,
5. global and detailed print intervals and number of segments for detailed dumps,
6. segments for which detailed dumps are to be saved,
7. intermediate dump segments,
8. by-pass options for detailed dumps.
9. mass balance/flux balance options

B1. Integration Procedure Solution Options

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50
INTGRTYP	NEGSLN	SLCOPT	ISMOLAR	ISMOLBCOPT

FORMAT(5I10)

INTGRTYP = integration procedure to be used for the simulation
= 1, explicit integration algorithm
= 3, split-time step algorithm
= 4, explicit integration using Smolarkiewicz corrector
= 5, leap-frog with Smolarkiewicz corrector
= 6, split-timestep with Smolarkiewicz corrector
(Note: options 3 and 6 are available only in the in-house version of RCA)

NEGSLN = option to permit the computation of negative concentrations
= 0, restrict concentrations to the positive plane (normal option)
= 1, permit the integration procedure to compute negative concentrations - used for special applications such as computing DO deficit or computing pH/alkalinity

SLCOPT = option for sigma-level correction for horizontal diffusion
= 0, no corrections will be applied
= 1, the sigma-level correction algorithm will be applied when computing horizontal fluxes

ISMOLAR = option for Smolarkiewicz correction
= 0, use 2nd order accurate Smolarkiewicz scheme
= 1, use recursive Smolarkiewicz scheme
ISMOLBCOPT = option for applying Smolarkiewicz correction schemes at boundaries
= 0, do not apply Smolarkiewicz scheme at boundaries
= 1, apply Smolarkiewicz scheme at boundaries

Normally, the user should select from either the explicit (INTGRTYP = 1 or 4) or the split-timestep algorithms (INTGRTYP=3 or 6) and positive solutions only (NEGSLN=0) options. Generally, by using the split-timestep option, the user can specify bigger timesteps for most segments within the model grid (only integrating a few critical segments with a small timestep) then could be chosen for explicit integration. It is strongly recommended that users not use option 5 for the reasons described previously. Usually either option 4 or 6 should be selected so as to reduce numerical dispersion (but at some cost in computational burden). The user can always evaluate the impact of numerical dispersion by running the model with and without Smolarkiewicz corrections and then comparing runs. For debugging purposes the user may wish to select INTGRTYP=1. When INTGRTYP is set equal to 1, the user may, for a particular segment, directly compute all of the terms of the derivative and compute the expected concentration at the next time level, via Equation 4:

$$c_i^{n+1} = c_i^n + \Delta t \left(\Sigma\, Q_{ji} c_j^n + \Sigma\, R_{ji} c_j^n - \Sigma \left(Q_{ik} + R_{ik} \right) c_i^n + W_i + K_i V_i c_i^n \right) \qquad (4)$$

where superscripts denote time levels in the integration and subscripts denote the model grid cells or segments.

The user should be aware that if NEGSLN is set equal to 0 and RCA computes a negative concentration for a segment (or group of segments) for a time-step, RCA will not let the concentration go negative. Rather, RCA will set the concentration for the next time-step to one quarter of the old concentration. Since this, in effect, results in adding mass to the system, RCA will print a warning message. If the number of occurrences of this corrective action is small and/or the mass being added to the system is small the user should not be too concerned. If, however, the number of warning messages and/or the mass being added to the system is large, the user should rerun the simulation using smaller time-steps for the critical period.

The choice of a value for ISMOLAR should be guided by experience and side-by-side comparisons. Generally use of the recursive version of the Smolarkiewicz corrector (ISMOLAR=1) provides for greater numerical accuracy, but at a cost of 30-50 percent increase in simulation run time. It may be possible to utilize the 2nd order accurate form of Smolarkiewicz (ISMOLAR=0) and reduce simulation run times, but the user should perform simulations using both options and compare results to see if the differences between schemes are acceptable.

The choice of applying either Smolarkiewicz correction scheme at the boundary should also be guided by experience and the frequency and quality of boundary condition data. For example, in tidal systems if data are only available on a monthly basis, it is probably better not to use Smolarkiewicz corrections at the boundary. If, however, for a tidal system where boundary conditions can be specified from hourly data (i.e., from continuous recorders) or from another model (as in the case of nested-models) the use of a Smolarkiewicz correction algorithm may be appropriate.

B2. Sigma-Level Correction Parameters (SLCOPT = 1)

A sigma-level grid may result in some undesired mixing in regions of steep topography. In some cases where the layers follow the river bottom or sea-bed of the water body, adjacent segments in the same layer can lie at significantly different depths in the vicinity of steep gradients. Because of this, "horizontal" diffusion between adjacent segments can result in an artificial vertical diffusion.

The numerical error caused by this can be reduced by using a correction method based on horizontally averaged concentrations. This method involves calculating the domain averages at user-specified standard depths, and performing horizontal mixing calculations using the divergence from the average instead of the actual concentration.

It is not necessary to specify the surface level (i.e., depth = 0) when specifying the standard level depths. If the surface depth is not specified, constituent values associated with the first sigma level are used for the surface values. To ensure proper interpolation from the standard levels back to the sigma levels, each bottom sigma level must be bracketed by two standard levels, i.e., it is required to specify a standard level depth greater than the maximum expected depth in sigma-level space.

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
IDTSLCSECS	TWARPSLC	NOSLC

FORMAT (FI10, 6X,A4,I10)

IDTSLCSECS = time interval between corrections (days)
TWARPSLC = time-warp or units used for IDTSLC. Normally IDTSLCSECS is in units of seconds. The user may, however, use different units.
= SECS or secs
= MINS or mins

NOSLC = number of standard levels

10	20		80
SLCDPTH(1)	SLCDPTH(2)	· · ·	SLCDPTH(NOSLC)

FORMAT (8F10.0)

SLCDPTH = standard-level depths

B3. Time Warp Scale Factor, Start of Simulation Time and Integration Interval for Kinetic Subroutine

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
TWARP	TZERO	IDTWQ

FORMAT(6X,A4,F10.0,I10)

TWARP = scale factor for integration step-size information. Normally the units for the general integration step-size, DT, and the kinetics integration step-size IDTWQ are seconds. However, the user may change the units of the input via TWARP.
= SECS or secs, DT and IDTWQ are read in seconds,
= MINS or mins, DT and IDTWQ are read in minutes,
= HRS or hrs, DT and IDTWQ are read in hours.

TZERO = prototype time for start of the simulation (days). Usually TZERO is set equal to 0.0, however, the user may start the simulation at a time greater than zero. For example, the user may wish to skip computing the winter months of a eutrophication model during the early calibration effort in order to reduce computer requirements. If the user has defined time equal to zero as January 1st and wishes to start the simulation in early May, TZERO would be set equal to 120. RCA would then ensure that all time-dependent inputs are at their proper starting values before initiating the simulation.

IDTWQ = integration interval for the kinetic subroutine (nominally in seconds). If IDTWQ = 0, RCA will integrate the kinetic portion of the derivative at the same timestep as used for the transport (see Card Group B4 below). If IDTWQ> 0, then the kinetic subroutine, TUNER, will be called every IDTWQ seconds. The latter implies that the kinetic portion of the derivative is assumed to be constant over the interval IDTWQ. (Note: the user should ensure that the value chosen for IDTWQ should be an exact multiple of any value of ISTEP or IDTSPLIT - see below).

The following inputs (B4 and B5) are required for INTGRTYP = 1, 4 or 5

B4. Number of Integration Step-Sizes (INTGRTYP = 1, 4, or 5)

For a number of water quality problems, there may be periods of time within the simulation period for which small integration steps are required (ex. during storm runoff events or spring snowmelt) versus times when larger timesteps can be used (ex. summer low flow). Therefore, RCA permits the user to specify a time-variable history of integration stepsizes to be used during the simulation.

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NSTEP

FORMAT(I10)

NSTEP = number of integration step-sizes to be read

B5. Integration Step-Size History (INTGRTYP = 1, 4, or 5)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40		70	80
ISTEP(1)	TBRK(1)	ISTEP(2)	TBRK(2)	- - -	ISTEP(NSTEP)	TBRK(NSTEP)

FORMAT (4(I10,F10.0))

ISTEP(I) = integration step-size (seconds)
TBRK(I) = time (days) until which ISTEP(I) is to be used, then switching to ISTEP(I+1) until TBRK(I+1)

The default units for ISTEP are seconds. However, if TWARP is specified as minutes, hours, or days then values for ISTEP will be in the same units as specified by TWARP. (Note: the value of ISTEP(I) should be an exact divisor of TBRK(I) for each ISTEP/TBRK pair and all ISTEP/TBRK pairs must be an exact divisor of IHYDDT - see C2 below).

The following input (B6) is required for INTGRTYP = 3 or 6

B6. Integration Stepsizes and Total Simulation Time (INTGRTYP = 3 or 6)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
IDTSPLIT	IDTFULL	TEND

FORMAT (2I10,F10.0)

IDTSPLIT = timestep to be used for the “high speed” or "critical" timestep segments (seconds)
IDTFULL = timestep to be used for remaining segments (seconds)
TEND = total simulation time, in days

The default units for IDTSPLIT and IDTFULL are seconds. However, if TWARP is specified as minutes, hours, or days then values for IDTSPLIT and IDTFULL will be in the same units as specified by TWARP. (Note: IDTSPLIT should be an exact divisor of IDTFULL and both IDTSPLIT and IDTFULL need to be an exact divisor of IHYDDT - see C2 below).

B7. Print Control Information

RCA permits two types of output dumps to be generated: global or domain-wide dumps at "coarse" time intervals, and detailed or selected segments at "fine" time intervals. By global dumps it is meant that the concentrations of all systems for all segments (i.e. all x, y, and z) are saved at the print interval, IPRNTG, described below. A note of caution: if a user has a 100 x 100 grid with 10 depth levels and 25 systems, a total of 10 Mbytes will be written at every IPRNTG interval. Clearly, one should not generate global dumps every day for a one year simulations (unless one has a disc storage system with large capacity).

However, in order to permit the user to generate daily (or hourly) output if necessary an option has been included in RCA to permit the user to select a number of segments for which information will be stored at a finer interval, IPRNTD, than is used for global dumps.

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60
IPRNTG	IPRNTD	NDMPS	TWARPP	IGDOPT	IDDOPT

FORMAT (3I10,6X,A4,2I10)

IPRNTG = time interval (default = seconds) for saving "global" (or grid-wide) concentrations,

IPRNTD = time interval (default = seconds) for saving "detailed" (or segment specific) concentrations and rate terms as per the user kinetic subroutine,

NDMPS = number of selected segments to be used in generating detailed dumps if IPRNTD$\neq$0

TWARPP = units in which IPRNTG and IPRNTD are input. Acceptable units for IPRNTG and IPRNTD are SECS (seconds), MINS (minutes), HRS (hours), or DAYS (days) and may be entered in either upper or lower case.
So, for example, a user who wished to get detailed dumps at one day intervals could specify IPRNTD = 86400, TWARPP = SECS or IPRNTD = 1, TWARPP = DAYS.

IGDOPT = global dump averaging option
= 0, write instantaneous (i.e., no averaging) concentrations or rates
= 1, write "averaged" concentrations or rates, using IPRNTG as the averaging interval

IDDOPT = detailed dump averaging option
= 0, write instantaneous (i.e., no averaging) concentrations or rates
= 1, write "averaged" concentrations or rates, using IPRNTD as the averaging interval

B8. <u>Segments for which Detailed Dumps are to be saved</u>
(Note: if IPRNTD = 0 or NDMPS = 0) skip this group and continue with B9.)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

4	8	12	---	72
IFDMPS(1,1)	IFDMPS(1,2)	IFDMPS(1,3)	---	IFDMPS(NDMP,3)

FORMAT (18I4)

IFDMPS(I,1) = X, Y and Z location designations, respectively, for the desired segments to be saved
IFDMP(I,2)
IFDMP(I,3)

B9. <u>System Bypass Options for Detailed Dumps</u>

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

2	4		80
DDMPBY(1)	DDMPBY(2)	---	DDMPBY(NOSYS)

FORMAT(40I2)

DDMPBY(ISYS) = system bypass options for making detailed dumps
= 0, include this system when making detailed dumps
= 1, do not include this system when making detailed dumps

This option permits the user to generate detailed dumps for a system even if that system is being bypassed (SYSBY=1) in the overall model computation. The major reason for including this option is so that users do not need to modify their GDP command decks if systems on being turned on and off during the calibration process. Of course, the user can also bypass making detailed dumps for a system (by setting DDMPBY=1), even if the system is being computed. However, the user should be sure to check whether the kinetic subroutine TUNER has been written in such a way as to make this input option function properly.

B10. <u>Segments to be Displayed for Intermediate Dumps</u>

RCA permits the user to monitor the progress of the water quality simulation by dumping the concentrations of six segments to the screen (or the user's output file with access via the UNIX/LINUX "tail" command) at each print interval during the simulation.

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

4	8	12	16	20	24		64	68	72
IX (1)	IY(1)	IZ(1)	IX (2)	IY(2)	IZ(2)	---	IX (6)	IY(6)	IZ(6)

FORMAT(18I4)

IX,IY,IZ = X, Y and Z IDs of segments to be displayed during the simulation.

B11. Mass Balance - Mass Flux Computation Options

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60
MASSBAL	IPRNTMB	TWARPMB	IMBOPT	ISTARTMB	IENDMB

FORMAT (2I10,6X,A4,3I10)

MASSBAL = mass/flux balance computation option
= 0, do not perform mass or flux balance computations
= 1, perform mass and flux balance computations

IPRNTMB = print interval (default = seconds) for saving mass balance and flux balance computations

TWARPMB = units in which IPRNTMB, ISTARTMB, and IENDMB are input. Acceptable units are SECS (seconds), MINS (minutes), HRS (hours), or DAYS (days).

IMBOPT = mass/flux balance dump averaging option
= 0, dump instantaneous (i.e., no averaging) mass balance and flux balance computations
= 1, dump "averaged" mass balance and flux balance computations, using IPRNTMB as the averaging interval

ISTARTMB = starting time (default = seconds) for beginning mass balance/flux balance computations
IENDMB = ending time (default = seconds) for performing mass balance/flux balance computations

This option permits the user to perform domain-wide mass/flux balance computations. The model output can be used to assess the importance of boundary inflows/outflows versus point, non-point, and atmospheric inputs, as well as to perform system-wide mass balance checks.

When selecting a "print interval" for applications in estuarine systems, it is recommended to select a print interval that is an exact multiple of a tidal cycle (44712 seconds or 12.42 hours). If one selects a non-tidal print interval it may make interpretation of flux balance results more difficult since the model would be outputting flux balances that occur over different parts of the tidal cycle and thus, for example, on a flood tide the model output would reflect a net import of mass into the model domain, while output on an ebb tide would reflect a net export of mass from the model domain. It is possible then in a tidal system where there is a small net export of mass from the domain that the flux balance would show a net import of mass if one were to start the flux balances at mean tide or mean tidal elevation but end the simulation at maximum flood tide. The user can also specify the starting and ending times, ISTARTMB and IENDMB, respectively, to help overcome this potential problem. (Example: if one were to perform a 365 day simulation, one could set ISTARTMB = 0 and then specify IENDMB = 31521960 seconds = 364.8375 days and the model will end at the same point in the tidal cycle.)

GROUP C: HYDRODYNAMIC TIME BREAKS AND SCALE FACTORS (STDIN)

Inputs required for this group include:

1. hydrodynamic file input options
2. time breaks for the hydrodynamic fields
3. flow and dispersion scale factors
4. file name containing the ECOMSED hydrodynamic fields

C1. Hydrodynamic File Input Options

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40
ICOLLOPT	HYDCYCOPT	LNDWTROPT	IDIFFOPT

FORMAT(4I10)

ICOLLOPT = option to inform RCA whether the gcm-geom and gcm_tran have been grid collapsed (i.e., the water quality model is a collapsed or aggregated version of the hydrodynamic grid)
= 0, no grid collapse was performed
= 1, grid collapse was performed

HYDCYCOPT = option to permit RCA to "cycle" or repeat the "gcm_tran" file, i.e. hydrodynamics are at periodic steady-state
= 0, do not "cycle" hydrodynamics if end-of-file encountered
= 1, "cycle" hydrodynamics, i.e., go back to beginning of the hydrodynamic file if end-of-file encountered

LNDWTROPT = option to select whether full-grid (land/water) hydrodynamic input to be read or just water cells
= 0, full-grid, i.e., land and water
= 1, just water cells (requires "wet-grid" input file from ECOMSED)

IDIFFOPT = option to specify and read "diffuser" files generated by ECOMSED
= 0, no diffuser files specified
= 1, diffuser files will be specified

The use of the HYDCYCOPT options permits users to perform water quality simulations for periods of time longer than the hydrodynamic model was run. For example, suppose a user wanted to run a 10 day simulation of a dye release into a tidal creek, subject to no freshwater inflow and with a constant tidal amplitude. The user could run the hydrodynamic model and save 10 days of periodic stage and velocity and set HYDCYCOPT = 0 , or just run the hydrodynamic model for one tidal cycle and save just one tidal cycle worth of stage and velocity and set, HYDCYCOPT = 1. RCA would go back to the beginning of the gcm_tran file (recycle) when the simulation time reached tidal cycle 1, 2, (day) etc. (Note: The use of HYDCYCOPT = 1 assumes that the hydrodynamics are at periodic steady-state.)

C2. Time Breaks for the Hydrodynamic Fields

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20
IHYDDT	UNITS

FORMAT(I10,6X,A4)

IHYDDT = averaging period used by ECOMSED to save hydrodynamic output (nominally in secs).

UNITS = time-warp or units used for IHYDDT. Normally IHYDDT is input in units of seconds. The user may, however, use different units:

= SECS or secs, IHYDDT is read in seconds,
= MINS or mins, IHYDDT is read in minutes,
= HRS or hrs, IHYDDT is read in hours.

C3. Dispersive Scale Factors

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
SCALRX	SCALRY	SCALRZ

FORMAT(3F10.0)

SCALRX = scale factor to multiply all horizontal or x-direction dispersion coefficients by

SCALRY = scale factor to multiply all lateral or y-direction dispersion coefficients by
SCALRZ = scale factor to multiply all vertical or z-direction dispersion coefficients by

Normally, SCALRX, SCALRY and SCALRZ should be set equal to 1.0.

C4. <u>The Number of Hydrodynamic and Diffuser Files</u>

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NOHYDFILNA

FORMAT (I10)

NOHYDFILNA = number of hydrodynamic and diffuser (if supplied by ECOMSED) files to be used in this simulation (maximum of 36)

C5. <u>The Names of the Files Containing the Hydrodynamic and Diffuser Transport Fields</u>

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

40	80
HYDFILNA	DIFFILNA

FORMAT(2A40)

HYDFILNA = complete path length and file name containing the ECOMSED transport and surface elevation data (gcm_tran)
ex.1 /usersb/neng0010/HYDRO/gcm_tran
ex.2 ../HYDRO/hydro.84
ex.3 ../HYDRO/hydro.85
(Note: the use of a "/" to specify the path or directory structure for a file is consistent with UNIX or

LINUX file naming structure. Running RCA under a WINDOWS environment means, of course (thanks to Bill Gates), using "\".

DIFFILNA = complete path length and file name containing the ECOMSED diffuser (or outfall) discharge information (gcm_gdiff).

GROUP D: INPUT FILE NAMES
(STDIN)

Inputs required for this group include:

1. the name of the file to be used to read boundary conditions inputs
2. the name of the file to be used to read point source loading inputs
3. the name of the file to be used to read nonpoint source loading inputs
4. the name of the file to be used to read fall-line loading inputs
5. the name of the file to be used to read atmospheric loading inputs
6. the name of the file to be used to read parameters, constants, miscellaneous time-variable functions and file names of miscellaneous files required by the users kinetic subroutine
7. the name of the file to be used to read initial conditions

RCA has been programmed so as to permit the user to develop a number of subfiles that contain RCA required inputs, rather than have all of the model input contained in one large input file as is done in AESOP. The reason for this is to provide the user with an extra degree of flexibility in generating model input files. If, for example, the user wishes to evaluate model response to a specific waste discharger, the user can set up two point source loading files, one with the discharger's load included and one with it not included. The user would then edit the standard input (STDIN) file and change the file name associated with the point source loadings (specified by D2) to the appropriate external point source file and then execute RCA. Since the standard input file (consisting of various input options for integration and printout histories and file names for the aforementioned RCA inputs) is so small, the time spent in editing should be very short. In addition, having various input groups permits users to develop a number of utility programs to generate the relevant input files rather than have one large complicated program to generate the entire input file at one time.

Further, as an option, the boundary condition, point source, etc. files may be read in either ASCII or binary (to save disc space) format. Binary format, of course, means that another FORTRAN program or utility must be used to generate the file. For binary files the user SHOULD NOT include the "comment" records in his or her input file.

New to RCA 3.0 is the option to bypass a particular file by specifying "NULL" or "null" (without the quotes) in the first four spaces. For example, if a particular application has no fall-line loads, the user just has to specify "NULL" for FLFILNA instead of having to create a dummy fall-line loads file with no loads.

D1. The Name of the File to be Used to Read Boundary Conditions Inputs, Binary Read Option

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

40 50
BCFILNA IBNRYOPT
FORMAT(A40, I10)

BCFILNA = complete path length and file name containing the boundary condition information (i.e., boundary segments and concentrations)
ex.1 /usersb/neng0010/HYDRO/boundcond (input file named "boundcond" resides in the /usersb/neng0010/HYDRO directory)
ex.2 bc.file (input file name bc.file resides in the current directory)
ex.3 ../inputs/bc.84 (input file named bc.84 resides in the inputs directory, which is a subdirectory of the directory one level above the currect directory)
= NULL to bypass this file. The appropriate vectors will be set to zero.

IBNRYOPT = option telling RCA to read ASCII or binary formatted boundary condition file
= 0, read ASCII file
= 1, read binary file

D2. The Name of the File to be Used to Read Point Source Loading Inputs, Binary Read Option

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

40 50
PSFILNA IBNRYOPT
FORMAT(A40,I10)

PSFILNA = complete path length and file name containing the point source loading information (loading segments and point source loads)
= NULL to bypass this file. The appropriate vectors will be set to zero.
IBNRYOPT = option telling RCA to read ASCII or binary formated file
= 0, read ASCII file
= 1, read binary file

D3. The Name of the File to be Used to Read Nonpoint Source Loading Inputs, Binary Read Option

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

40	50
NPSFILNA	IBNRYOPT

FORMAT(A40,I10)

NPSFILNA = complete path length and file name containing the nonpoint source loading information (loading segments and nonpoint source loads)
= NULL to bypass this file. The appropriate vectors will be set to zero.
IBNRYOPT = option telling RCA to read ASCII or binary formated files
= 0, read ASCII file
= 1, read binary file

D4. The Name of the File to be Used to Read Fall-line Loading Inputs, Binary Read Option

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

40	50
FLFILNA	IBNRYOPT

FORMAT(A40,I10)

FLFILNA = complete path length and file name containing the fall-line loading information (fall-line segments and fall-line loads)
= NULL to bypass this file. The appropriate vectors will be set to zero.
IBNRYOPT = option telling RCA to read ASCII or finary formatted file
= 0, read ASCII file
= 1, read binary file

D5. The Name of the File to be Used to Read Atmospheric Loading Inputs, Binary Read Option

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

40	50
ATMFILNA	IBNRYOPT

FORMAT(A40,I10)

ATMFILNA = complete path length and file name containing the atmospheric loading information (amtospheric loads)
= NULL to bypass this file. The appropriate vectors will be set to zero.
IBNRYOPT = option telling RCA to read ASCII or binary formated file
= 0, read ASCII file
= 1, read binary file

D6. The Name of the File to be Used to Read Parameters, Constants, Time-Variable Functions and Miscellaneous File Names, Binary Read Option

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

40	50
PCFILNA	IBNRYOPT

FORMAT(A40,I10)

PCFILNA = complete path length and file name containing the parameters, constants and time-variable functions

= NULL to bypass this file. The appropriate vectors will be set to zero.

IBNRYOPT = option telling RCA to read ASCII or binary formatted files
= 0, read ASCII file
= 1, read binary file

D7. The Name of the File to be Used to Read Initial Conditions, Binary Read Option

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

40	50
ICFILNA	IBNRYOPT

FORMAT(A40,I10)

ICFILNA = complete path length and file name containing the initial conditions

IBNRYOPT = option telling RCA to read ASCII or binary formatted files
= 0, read ASCII file
= 1, read binary file

GROUP E: STABILITY AND ACCURACY CRITERIA (STDIN)

E1. Stability Criteria

80
Comment
FORMAT(A80)

Comment = Comment line (ignored by RCA)

20 30 80
CMAX(1) CMAX(2) - - - CMAX(NOSYS)
FORMAT(10X,7F10.0)

CMAX(ISYS) = stability criteria for system ISYS, i.e. a maximum concentration that if exceeded in any segment or grid cell indicates that the numerical integration procedure has become unstable. If an instability occurs an appropriate error message is written and the simulation is terminated.

E2. Minimum Concentrations for Numerical Integration

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

20 30 80
CMIN(1) CMIN(2) - - - CMIN(NOSYS)
FORMAT(10X,7F10.0)

CMIN(ISYS) = the minimum concentration or "floor" for system ISYS. As was mentioned earlier, under the description of the input variable NEGSLN, RCA normally does not permit negative solutions to occur. It does this by "quartering" concentrations. If, however, enough "quartering" of concentrations occur in a segment, underflows (i.e., concentrations less than 1.0E-38) may occur, which will result in the RCA run terminating. To prevent this the user should specify minimum values which will limit the "quartering" process. Recommended values for CMIN are 1.0E-20.

GROUP F: END OF SIMULATION DUMPS
(STDIN)

Inputs from this group are read at the end of a simulation run.

F1. System Dumps

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

At the completion of the simulation the user may wish to display or dump the concentrations of any or all segments for any or all systems. The following inputs are read for each global dump saved starting with the first and going through system dump = NGDMP (where NGDMP is set in the users kinetic subroutine).

3	6	9	12		69	72	75	78	80
IVAR	IX(1)	IY(1)	IZ(1)	- - -	IX(8)	IY(8)	IZ(8)	LYRDMP	LYR

FORMAT(I3,24I3,A3,I2)

IVAR = 1, for global system dumps (Note: currently only the state-variable concentrations are available for dumping, hence IVAR = 1. However, in the future, RCA may permit IVAR may take on other values.)
IX,IY,IZ = x, y and z designation for the segment to be displayed
LYRDMP = if LYRDMP is read in as "LYR" then all segments within a particular layer (for layer = LYR) will be displayed without the user being required to specify each IX,IY,IZ combination
LYR = the layer for which concentrations are to be dumped (if LYRDMP is read as "LYR")

Table 4 presents an example of the STDIN input file for Groups A through F.

TABLE 4. EXAMPLE OF STANDARD INPUT FILE - STDIN

```
C    Cycle List_Geom  List_BCs  List_WKs  List_PCs  List_ICs   IDIAGDT    INPCHK
         0         0         0         0         0         0         0         0
C    Model Run Descriptor Comments Follow (Terminate with an "END")
  MERL Tank Simulation
  Input set up to simulate Control Tanks 0 - 5 - 8
END
C    System Names (1 ... NOSYS)
     SAL   PHYT1   PHYT2    RPOP    LPOP    RDOP    LDOP     DIP    RPON    LPON
    RDON    LDON     NH3    NO23     SIU      SI    RPOC    LPOC    RDOC    LDOC
   REDOC   EXDOC    O2EQ      DO
C    Type of Simulation
TIME-VARIABLE SIMULATION
C    System By-pass Options (1 ... NOSYS)
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
C INTGRTYP    NEGSLN    SLCOPT   ISMOLAR ISMOLBCOP
         1         0         0         0         0
C    TWARP     TZERO IDTWQSECS
      MINS       0.0         0
C    NSTEP
         1
CIntg_Step UntilTime Intg_Step UntilTime Intg_Step UntilTime Intg_Step UntilTime
        72      109.     1090.
C    PRNTG     PRNTD     NDMPS    TWARPP    IGDOPT    IDDOPT
       240       240         3       HRS         0         0
C    Detailed Dumps (IR,IC,IL)  (1 ... NDMPS)
   2   2   1   2   2   2   2   1   1
C    Detailed Dump By-pass Options (1 ... NOSYS)
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
C    Intermediate Dumps (IR,IC,IL)  (1 ... 6)
   2   2   1   2   2   2   2   2   1   2   2   2   2   2   1   2   2   2
C  MASSBAL   IPRNTMB   TWARPMB    IMBOPT ISTARTMB    IENDMB
         1    447120      SECS         0        0  31521960
C ICOLLOPT HYDCYCOPT LNDWTROPT
        0         0        1      non-collapsed, non-split hydro files,water only
C   IHYDDT     UNITS
       720       HRS
C   SCALRX    SCALRY    SCALRZ
       1.0       1.0     1.000
C   Number and Names of Hydrodynamic Files
         2
gcm_tran_1-6
gcm_tran_7-12
C    Boundary Condition File Name      Binary Read Option
bc058.inp
C    Point Source Loads File Name      Binary Read Option
NULL
C    Non-point Source Loads File Name  Binary Read Option
NULL
C    Fall-line Loads File Name         Binary Read Option
fltest.inp
C    Atmospheric Loads File Name       Binary Read Option
NULL
C    Params, Consts, TVFs File Name    Binary Read Option
pctvf058.inp
C    Initial Conditions File Name      Binary Read Option
ic058.inp
C    Stability Concentrations
stability      5000.     3000.    3000.0    1000.0   100.000      20.0     50.00
              100.00     500.0    100.00    1000.0     500.0    1000.0    1000.0
              1000.0    1000.0    1000.0    1000.0    2000.0    5000.0    3000.0
              1000.0    3000.0    5000.0
C    Floor Concentrations
floor       0.000001  0.000001  0.000001  0.000001  0.000001  0.000001  0.000001
            0.000001  0.000001  0.000001  0.000001  0.000001  0.000001  0.000001
            0.000001  0.000001  0.000001  0.000001  0.000001  0.000001  0.000001
            0.000001  0.000001  0.000001
C   Selection of Simulation Dumps Follow
  1                                                                     LYR  1
  1                                                                     LYR  2
                                                                            End Sys  1
  1                                                                     LYR  1
  1                                                                     LYR  2
                                                                            End Sys  2
/*
```

GROUP G: BOUNDARY CONCENTRATIONS (BCFILNA)

The user may choose to input boundary condition information using either sigma-level specification or standard-level specification. For sigma-level specification the user enters the boundary concentrations associated with each boundary segment in the model, specifying both the (IX,IY,IZ) segment location and the average water column concentration at the appropriate model segment depth. For example, assume one is modeling a river with one upstream and one downstream boundary, using a one column wide (i.e. laterally averaged) grid and five equally spaced vertical layers. Then the model has a total of ten boundary conditions, one boundary condition for each of the five upstream layers and one for each of the five downstream layers. If the total depth of the upstream boundary is 5 meters, then the boundary conditions would be assumed to represent water quality conditions every one meter in depth. If the total depth at the downstream boundary is 15 meters, then the boundary conditions would be assumed to represent water quality conditions every three meters in depth.

For standard level specifation, the user first specifies the standard levels (or depths) at which the boundary conditions will be provided for a particular system and then specifes for each (IX,IY) boundary location the number of standard level depths for this location and the associated water column concentrations at the standard levels or depths. RCA will then interpolate (using linear interpolation) the specified standard level boundary conditions onto the sigma-level grid. Using the same river system model as above, and having water column observations only at the surface, 3 meter, 10 meter and 15 meter depths, the user would specify four standard level depths, i.e. 0, 3, 10 and 15 meters, and two boundary (IX,IY) locations (i.e., the (IX,IY) locations of the upstream and downstream boundaries). For the upstream boundary, data are available for only two standard levels, 0 and 3 meters, while for the downstream boundary the user would input water quality concentrations at the four standard levels, 0, 3, 10 and 15 meters. RCA would then interpolate the two upstream concentrations, using linear interpolation, to equivalent sigma-level depths of 0.5, 1.5, 2.5, 3.5 and 4.5 meters, and would also interpolate the four downstream concentrations onto the downstream sigma-level depths of 1.5, 4.5, 7.5, 10.5, and 13.5 meters.

Inputs required for this group include:

1. boundary condition input options
2. number of boundary conditions
3. scale factor for boundary concentrations
4. actual boundary concentrations

G1. Boundary Condition Input Option

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 20
IBCOPT IBCPWLOPT
FORMAT(2I10)

IBCOPT = input option
= 1, time-invariant (or constant) sigma-level concentrations will be read
= 2, time-variable sigma-level boundary concentrations will be read
= 3, time-invariant (or constant) standard level concentrations will be read
= 4, time-variable standard level boundary concentrations will be read

IBCPWLOPT = option to select step-function or piecewise linear interpolation of time-variable boundry conditions.
= 0, step-function interpolation will be used
= 1, piecewise linear interpolation will be used

The remaining boundary condition input is dependent upon the IBCOPT input option chosen. Data inputs for sigma-level option 1 (constant concentrations) and option 2 (time-variable) will be presented first, followed by data inputs associated with standard level options 3 (constant concentrations) and option 4 (time-variable).

Constant or Time-Invariant Concentrations - Sigma Level (IBCOPT = 1)

Data associated with Data Types G2, G3 and G4 will be read NOSYS times; once for each system in the model.

G2. Number of Boundary Conditions

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

```
        10
NOBC(ISYS)
FORMAT(I10)
```

NOBC(ISYS) = the number of boundary conditions for system ISYS

(Note: If there are no boundary conditions to be specified for a system (NOBC = 0) then no input is required for G3 or G4; just continue with next G2.)

G3. Boundary Concentration Scale Factor

```
              80
         Comment
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
          10
SCALBC(ISYS)
FORMAT(F10.0)
```

SCALBC(ISYS) = scale factor for system ISYS

Normally SCALBC(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in boundary inputs, SCALBC(ISYS) would then be set equal to 0.75.

G4. Boundary Segments and Boundary Concentrations

```
              80
         Comment
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
          10          14          17          20
BBC(1,ISYS) IBC(1,1,ISYS) IBC(2,1,ISYS) IBC(3,1,ISYS)  - - -

             70               74                77                80
  BBC(NOBC,ISYS) IBC(1,NOBC,ISYS) IBC(2,NOBC,ISYS) IBC(3,NOBC,ISYS)
FORMAT(4(F10.0,1X,3I3))
```

BBC(I,ISYS) = boundary concentration (mg/L)
IBC(1,I,ISYS) = x-cell number of boundary condition grid element

IBC(2,I,ISYS) = y-cell number of boundary condition grid element
IBC(3,I,ISYS) = z-cell or layer number of boundary condition grid element

The following example illustrates how to assign the x, y and z information required for RCA.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L
2	L	OWB			L	L	L						L	L	L
3	L	OWB								L				FFI	L
4	L	OWB								L	L			L	L
5	L	OWB											L	L	L
6	L	L	L	L	L	L	L	L	FFI	L	L	L	L	L	L

The above illustration shows a 15x6 grid; NX=15 and NY=6. Grid elements denoted by an "L" indicate either a land segment or the limits of the model domain. Grid elements denoted by "OWB" indicate an open water boundary (including flow and dispersion consistent with the ECOMSED grid notation), while those represented by "FFI" represent free flowing inputs (flow only, no dispersion), such as a river/dam or an onshore outfall/intake discharge. The model also has 6 vertical layers.

The model, then, has 36 ((4 OWB + 2 FFI)*6) boundary conditions, specified as follows:

IBC(1,I,ISYS)	IBC(2,I,ISYS)	IBC(3,I,ISYS)
2	2	1
2	2	2
:	:	:
2	2	6
2	3	1
:	:	:
2	3	6
2	4	1
:	:	:
2	4	6
2	5	1
:	:	:
2	5	6
9	6	1
:	:	:
9	6	6
14	3	1
:	:	:
14	3	6

Time-Variable Concentrations - Sigma Level (IBCOPT = 2)

G2. Time for which Boundary Concentrations are being Specified

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

20	30
NXBCTSECS	TWARPBC

FORMAT (10X,I10,6XA4)

NXBCTSECS = time in seconds (or units specified by TWARPBC)
TWARPBC = time-warp or units used for NXBCTSECS.
Normally NXBCTSECS is input in units of seconds. The user may, however, use different units.
= SECS or secs,
= MINS or mins,
= HRS or hrs,
= DAYS or days.

Data associated with Data Types G3 through G6 will be read NOSYS times; once for each system in the model.

G3. Number of Boundary Conditions

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NOBC(ISYS)

FORMAT(I10)

NOBC(ISYS) = the number of boundary conditions for system ISYS

(Note: If there are no boundary conditions to be specified for a system (NOBC = 0), then no input is required for G4, G5 or G6; just continue with next G3.)

G4. Boundary Concentration Scale Factor

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALBC(ISYS)

FORMAT(F10.0)

SCALBC(ISYS) = scale factor for system ISYS

Normally SCALBC(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in boundary inputs, SCALBC(ISYS) would then be set equal to 0.75.

G5. Boundary Segments

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

14	17	20	
IBC(1,1,ISYS)	IBC(2,1,ISYS)	IBC(3,1,ISYS)	- - -

74	77	80
IBC(1,NOBC,ISYS)	IBC(2,NOBC,ISYS)	IBC(3,NOBC,ISYS)

FORMAT(10X,7(I4,I3,I3))

IBC(1,I,ISYS) = x-cell number of boundary condition grid element
IBC(2,I,ISYS) = y-cell number of boundary condition grid element
IBC(3,I,ISYS) = z-cell or layer number of boundary condition grid element

G6. Boundary Concentrations

20	30		80
BBC(1,ISYS)	BBC(2,ISYS)	---	BBC(NOBC(ISYS),ISYS)

FORMAT(10X,7F10.0)

BBC(I,ISYS) = boundary concentration (mg/L)

The boundary concentrations (BBC) should be specified in the same order as the x, y, and z (IBC) designations were read. After input types G3 through G6 are repeated for each system, then the simulation time at which the next set of boundary concentrations is to be read, NXBCT, is specified; followed by the next set of boundary concentrations (input type G6); it is not necessary to repeat input types G3, G4 and G5. If NOBC(ISYS) = 0 for system ISYS then the user would skip specifying G6 input data for that system.

Data associated with Data Types G3, G4, G5 and G6 will be read NOSYS times; once for each system in the model.

Constant or Time-Invariant Concentrations - Standard Level (IBCOPT = 3)

G2. Number of Boundary Conditions

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NOBC(ISYS)
FORMAT(I10)

NOBC(ISYS) = the number of boundary conditions for system ISYS

(Note: If there are no boundary conditons to be specified for a system (NOBC = 0), then no input is required for G3, G4, G5, G6 or G7; just continue with next G2.)

G3. Boundary Concentration Scale Factor

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALBC(ISYS)
FORMAT(F10.0)

SCALBC(ISYS) = scale factor for system ISYS

Normally SCALBC(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in boundary inputs, SCALBC(ISYS) would then be set equal to 0.75.

G4. Number of Standard Level Depths

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5
NLVLS(ISYS)

FORMAT(I5)

NLVLS(ISYS) = the maximum number of standard level depths required for system ISYS

G5. Standard Level Depths

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

20	30	80
SLDEPTH(1,ISYS)	SLDEPTH(2,ISYS)	--- SLDEPTH(NLVLS,ISYS)

FORMAT(10X,7F10.0)

SLDEPTH(I,ISYS) = the depth of standard level I, (meters) to be used to specify boundary concentration data for system ISYS

G6. Boundary Segments and Number of Standard Levels to be Read

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5	10	15
IBCSL(1,IBC,ISYS)	IBCSL(2,IBC,ISYS)	NOBCSL(IBC,ISYS)

FORMAT(3I5)

IBCSL(1,IBC,ISYS) = x-cell number of boundary condition segment
IBCSL(2,IBC,ISYS) = y-cell number of boundary condition segment
NOBCSL(IBC,ISYS) = number of standard level concentrations to be read for boundary condition IBC (maximum number must be less than or equal to NLVLS)

G7. Boundary Concentrations at Standard Levels

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

20	30	80
SLBC(1,IBC,ISYS)	SLBC(2,IBC,ISYS) —	SLBC(NOBCSL,IBC,ISYS)

FORMAT(10X,7F10.0)

SLBC(I,IBC,ISYS) = boundary concentration (mg/L)

After reading in the boundary concentrations at the standard levels RCA will perform a linear interpolation of the input data onto the sigma level grid and produce a set of boundary segment numbers (IX,IY and IZ) and concentrations similiar to the input required for IBCOPT = 1.

Inputs G4, G5, G6, and G7 will be read NOBC(ISYS) times; once for each boundary condition

Time-Variable Conditions - Standard Level (IBCOPT = 4)

G2. Time for which Boundary Concentrations are being Specified

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

20	30
NXBCTSECS	TWARPBC

FORMAT (10X, I10,6X,A4)

NXBCTSECS = time in seconds (or units specified by TWARPBC)
TWARPBC = units to be used for NXBCTSECS
= SECS or secs,
= MINS or mins,
= HRS or hrs,
= DAYS or days.

Data associated with Data Types G3 through G8 will be read NOSYS times; once for each system in the model.

G3. Number of Boundary Conditions

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NOBC(ISYS)

FORMAT(I10)

NOBC(ISYS) = the number of boundary conditions for system ISYS

(Note: If there are no boundary conditons to be specified for a system (NOBC = 0), then no input is required for G4 to G8; just continue with next G3.)

G4. Boundary Concentration Scale Factor

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALBC(ISYS)
FORMAT(F10.0)

SCALBC(ISYS) = scale factor for system ISYS

Normally SCALBC(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in boundary inputs, SCALBC(ISYS) would then be set equal to 0.75.

G5. Number of Standard Level Depths

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NLVLS(ISYS)
FORMAT(I10)

NLVLS(ISYS) = the maximum number of standard level depths required to specify boundary concentration information for system ISYS

G6. Standard Level Depths

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

20 30 80
SLDEPTH(1,ISYS) SLDEPTH(2,ISYS) --- SLDEPTH(NLVLS,ISYS)
FORMAT(10X,7F10.0)

SLDEPTH(I,ISYS) = the depth of standard level I, (meters)

G7. Boundary Segments and Number of Standard Levels to be Read

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

5 10 15
IBCSL(1,IBC,ISYS) IBCSL(2,IBC,ISYS) NOBCSL(IBC,ISYS)
FORMAT(3I5)

IBCSL(1,IBC,ISYS) = x-cell number of boundary condition segment
IBCSL(2,IBC,ISYS) = y-cell number of boundary condition segment
NOBCSL(IBC,ISYS) = number of standard level concentrations to be read for boundary condition IBC (maximum number must be less than or equal to NLVLS)

G8. Boundary Concentrations at Standard Levels

20 30 80
SLBC(1,IBC,ISYS) SLBC(2,IBC,ISYS) — SLBC(NOBCSL,IBC,ISYS)
FORMAT(10X,7F10.0)

SLBC(I,IBC,ISYS) = boundary concentration (mg/L)

After reading in the boundary concentrations at the standard levels RCA will perform a linear interpolation of the input data onto the sigma level grid and produce a set of boundary segment numbers (IX,IY and IZ) and concentrations similiar to the input required for IBCOPT = 2.

After input types G2 through G8 are read for each system, then the time of the next set of boundary concentrations, NXBCT, will be required; followed by the next set of boundary concentrations specified at standard levels (input type G8); it is not necessary to repeat input types G2 through G7.

Table 5 presents an example of a boundary condition input file using time- variable sigma level input (IBCOPT = 2), while Table 6 presents an example of a boundary condition input file using time-invariant or constant standard level input.

TABLE 5. EXAMPLE OF TIME-VARIABLE SIGMA-LEVEL BOUNDARY CONDITIONS - BCFILNA

```
C    BCOPT    PWLOPT
         2         0            base values - no additions to PO4,NH3,Si for algal biomass
C          NXBCTSECS   TWARPBC
                   0      DAYS      time  JAN 1 ,81
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 1salinity .3070E+02 .3070E+02
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 2Wint Phy .1750E+00 .1750E+00
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 3Summ Phy .5250E-01 .5250E-01
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 4 RPOP    .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 5 LPOP    .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 6 RDOP    .1000E-02 .1000E-02
C     NOBC
         2                           no. of boundary condition segments

C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 7 LDOP    .4000E-02 .4000E-02
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 8Tot PO4  .3844E-01 .3844E-01
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
 9 RPON    .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
10 LPON    .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
11 RDON    .1000E-02 .1000E-02
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
12 LDON    .8000E-02 .8000E-02
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
13 Tot NH4 .7062E-01 .7062E-01
```

TABLE 5. EXAMPLE OF TIME-VARIABLE SIGMA-LEVEL BOUNDARY CONDITIONS - BCFILNA (Cont.)

```
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
14 NO23    .1050E+00 .1050E+00
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
15 BioG Si .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
16 TOT SI  .2413E+00 .2413E+00
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
17 RPOC    .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
18 LPOC    .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
19 RDOC    .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
20 LDOC    .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor

C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
21 REDOC   .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
22 EXDOC   .1000E-05 .1000E-05
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
23 AQ SOD  .0000E+00 .0000E+00
C     NOBC
         2                           no. of boundary condition segments
C   SCALBC
       1.0                          scale factor
C         LOCATIONS OF BOUNDARY SEGMENTS
 bc segs     2  1  1   2  1  2
24 DO      .1141E+02 .1141E+02
                  31      time  FEB 1   81
 1salinity .3000E+02 .3000E+02
 2wint phy .2350E+00 .2350E+00
 3summ phy .4050E-01 .4050E-01
 4rpop     .1000E-05 .1000E-05
 5lpop     .1000E-05 .1000E-05
 6rdop     .1000E-02 .1000E-02
 7ldop     .4000E-02 .4000E-02
 8po4 tot  .3581E-01 .3581E-01
 9rpon     .1000E-05 .1000E-05
10 lpon    .1000E-05 .1000E-05
11 rdon    .1000E-02 .1000E-02
12 ldon    .8000E-02 .8000E-02
13 nh3 tot .7545E-01 .7545E-01
14 no23    .1060E+00 .1060E+00
15 bio si  .1000E-05 .1000E-05
16 tot si  .2919E+00 .2919E+00
17 rpoc    .1000E-05 .1000E-05
```

TABLE 5. EXAMPLE OF TIME-VARIABLE SIGMA-LEVEL BOUNDARY CONDITIONS - BCFILNA (Cont.)

```
18 lpoc     .1000E-05 .1000E-05
19 rdoc     .1000E-05 .1000E-05
20 ldoc     .1000E-05 .1000E-05
21 redoc    .1000E-05 .1000E-05
22 exdoc    .1000E-05 .1000E-05
23 aq sod   .0000E+00 .0000E+00
24 do       .1284E+02 .1284E+02
                  59        time  MAR 1       81
 1salinity .2940E+02 .2940E+02
 2wint phy .2300E+00 .2300E+00
 3summ phy .7350E-01 .7350E-01
 4rpop      .1000E-05 .1000E-05
 5lpop      .1000E-05 .1000E-05
 6rdop      .1000E-02 .1000E-02
 7ldop      .4000E-02 .4000E-02
 8po4 tot   .2241E-01 .2241E-01
 9rpon      .1000E-05 .1000E-05
10 lpon     .1000E-05 .1000E-05
11 rdon     .1000E-02 .1000E-02
12 ldon     .8000E-02 .8000E-02
13 nh3 tot  .7067E-01 .7067E-01
14 no23     .3150E-01 .3150E-01
15 bio si   .1000E-05 .1000E-05
16 tot si   .1497E+00 .1497E+00
17 rpoc     .1000E-05 .1000E-05
18 lpoc     .1000E-05 .1000E-05
19 rdoc     .1000E-05 .1000E-05
20 ldoc     .1000E-05 .1000E-05
21 redoc    .1000E-05 .1000E-05
22 exdoc    .1000E-05 .1000E-05
23 aq sod   .0000E+00 .0000E+00
24 do       .1173E+02 .1173E+02
                  90       time  APR 1     81
 1salinity .2780E+02 .2780E+02
 2wint phy .1300E+00 .1300E+00
 3summ phy .6900E-01 .6900E-01
          //////////
   This portion of input file,
   covering the period from April
   through Oct is not being shown
          //////////
21 redoc    .1000E-05 .1000E-05
22 exdoc    .1000E-05 .1000E-05
23 aq sod   .0000E+00 .0000E+00
24 do       .7260E+01 .7260E+01
                 304        time  NOV 1      81
 1salinity .3050E+02 .3050E+02
 2wint phy .7000E-01 .7000E-01
 3summ phy .2100E-01 .2100E-01
 4rpop      .1000E-05 .1000E-05
 5lpop      .1000E-05 .1000E-05
 6rdop      .1000E-02 .1000E-02
 7ldop      .4000E-02 .4000E-02
 8po4 tot   .5298E-01 .5298E-01
 9rpon      .1000E-05 .1000E-05
10 lpon     .1000E-05 .1000E-05
11 rdon     .1000E-02 .1000E-02
12 ldon     .8000E-02 .8000E-02
13 nh3 tot  .9555E-01 .9555E-01
14 no23     .9150E-01 .9150E-01
15 bio si   .1000E-05 .1000E-05
16 tot si   .3718E+00 .3718E+00
17 rpoc     .1000E-05 .1000E-05
18 lpoc     .1000E-05 .1000E-05
19 rdoc     .1000E-05 .1000E-05
20 ldoc     .1000E-05 .1000E-05
21 redoc    .1000E-05 .1000E-05
22 exdoc    .1000E-05 .1000E-05
23 aq sod   .0000E+00 .0000E+00
24 do       .8015E+01 .8015E+01
                 335        time  DEC 1      81
 1salinity .3060E+02 .3060E+02
 2wint phy .2300E+00 .2300E+00
 3summ phy .6900E-01 .6900E-01
 4rpop      .1000E-05 .1000E-05
 5lpop      .1000E-05 .1000E-05
 6rdop      .1000E-02 .1000E-02
 7ldop      .4000E-02 .4000E-02
 8po4 tot   .3999E-01 .3999E-01
 9rpon      .1000E-05 .1000E-05
10 lpon     .1000E-05 .1000E-05
11 rdon     .1000E-02 .1000E-02
12 ldon     .8000E-02 .8000E-02
13 nh3 tot  .7923E-01 .7923E-01
14 no23     .1010E+00 .1010E+00
15 bio si   .1000E-05 .1000E-05
16 tot si   .2403E+00 .2403E+00
17 rpoc     .1000E-05 .1000E-05
18 lpoc     .1000E-05 .1000E-05
19 rdoc     .1000E-05 .1000E-05
20 ldoc     .1000E-05 .1000E-05
21 redoc    .1000E-05 .1000E-05
22 exdoc    .1000E-05 .1000E-05
23 aq sod   .0000E+00 .0000E+00
24 do       .9500E+01 .9500E+01
                 366.0000      time JAN 1, 82 — end of simulation
```

TABLE 6. EXAMPLE OF TIME-INVARIANT STANDARD LEVEL BOUNDARY CONDITION INPUT - BCFILNA

```
C   IBCOPT   IBCLOPT
         4         0
C     NOBC
        14
C   SCALBC  - scale factor
        1.
C    NLVLS  - No of Std Lvl Depths
         4
C  Standard Level Depths
  SLDPTHS       0.00     20.00     60.00    110.00
C  BC Locations/# of Stardard Level Data to read (IX,IY,NSTLVLS)
  Salinity  19  6  4  19  7  4  19  8  4  19  9  4  19 10  4  19 11  4  19 12  4
            19 13  4  19 14  4  19 15  4  19 16  4  19 17  4  19 18  4  19 19  4
C Salinity boundary condition data for each standard level
   19, 6  0.3240E+020.3240E+020.3250E+020.3250E+02
   19, 7  0.3240E+020.3240E+020.3250E+020.3250E+02
   19, 8  0.3240E+020.3240E+020.3250E+020.3250E+02
   19, 9  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,10  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,11  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,12  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,13  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,14  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,15  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,16  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,17  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,18  0.3240E+020.3240E+020.3250E+020.3250E+02
   19,19  0.3240E+020.3240E+020.3250E+020.3250E+02
C     NOBC
        14
C   SCALBC  - scale factor
        1.
C    NLVLS  - No of Std Lvl Depths
         4
C  Standard Level Depths
  SLDPTHS       0.00     20.00     60.00    110.00
C  BC Locations/# of Stardard Level Data to read (IX,IY,NSTLVLS)
  Phyto1    19  6  4  19  7  4  19  8  4  19  9  4  19 10  4  19 11  4  19 12  4
            19 13  4  19 14  4  19 15  4  19 16  4  19 17  4  19 18  4  19 19  4
C Phytoplankton - Algal Group 1 boundary condition data for each standard level
   PHYT1  0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
          0.2000E-010.1500E-010.1000E-010.5000E-02
C     NOBC
        14
C   SCALBC  - scale factor
        1.
C    NLVLS  - No of Std Lvl Depths
         4
C  Standard Level Depths
  SLDPTHS       0.00     20.00     60.00    110.00
C  BC Locations/# of Stardard Level Data to read (IX,IY,NSTLVLS)
  Phyto2    19  6  4  19  7  4  19  8  4  19  9  4  19 10  4  19 11  4  19 12  4
            19 13  4  19 14  4  19 15  4  19 16  4  19 17  4  19 18  4  19 19  4
C Phytoplankton - Algal Group 2 boundary condition data for each standard level
  PHYT2   0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
          0.5000E-020.5000E-020.2000E-020.2000E-02
            //////////
            rest of boundary input not displayed

            //////////
```

GROUP H: POINT SOURCE LOADS
(PSFILNA)

Inputs required for this group include:

1. point source loads input option
2. index table of point source loads
3. number of point source loads
4. scale factor for point source loads
5. actual point source loads

H1. Point Source Loads Input Option

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20
IPSOPT	IPSPWLOPT

FORMAT (2I10)

IPSOPT = input option
= 1, all point source loads are constant in time
= 2, time-variable point source loads will be used
IPSPWLOPT = option to select step-function or piecewise linear interpolation of time-variable point source loadings.
= 0, step-function interpolation will be used
= 1, piecewise linear interpolation will be used

The remaining point source loads inputs are dependent upon the IPSOPT input option chosen. Data inputs for option 1 (constant loads) will be presented first, followed by data inputs associated with option 2 (time-variable).

H2. Index Table of Point Source Loads

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5	10	15	65
IPS(1,I,ISYS)	IPS(2,I,ISY)	IPS(3,I,ISYS)	LOCATION

FORMAT (3I5,A50)

IPS(1,I,ISYS) = load identifier (should be numbered consecutively from 1 through the number of point source loads included in the model
= -99 to signal end of input
IPS(2,I,ISYS) = the x-cell number of the point source load
IPS(3,I,ISYS) = the y-cell number of the point source load.
LOCATION = a 50-character alpha-numeric description of the point source load locations, ex. Blue Plains WWTP

16	22		70
ZFRACPS(1,I)	ZFRACPS(2,I)	. . .	ZFRACPS(NZ,I)

FORMAT (10X,10F6.3)

ZFRACPS(1,I) = fraction of point source load discharged to layer 1,2, . . ., through NZ (note: fractions should sum up to 1.0)
:
ZFRACPS(NZ,I) If a user wished to distribute a load equally throughout the water column and if NZ=10, then ZFRACPS(1,I) through ZFRACPS(10,I) would each be set to 0.1. If a user wished to put a load in the bottom two cells only (and again if NZ=10), then ZFRACPS(1,I) through ZFRACPS(8,I) = 0.0, and ZFRACPS(9,I) = ZFRACPS(10,I) = 0.5

<u>Constant or Time-Invariant Loads (IPSOPT = 1)</u>

Data associated with Data Types H3, H4 and H5 will be read NOSYS times; once for each system in the model.

H3. <u>Number of Point Source Loads</u>

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NOPS(ISYS)

FORMAT(I10)

NOPS(ISYS) = the number of point source loads for system ISYS

(Note: If there are no point source loads to be specified for a system (NOPS = 0), then no input is required for H4 or H5; just continue with next H3.

H4. Point Source Load Scale Factor

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALPS(ISYS)
FORMAT(F10.0)

SCALPS(ISYS) = scale factor system ISYS

Normally SCALPS(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in point source inputs, SCALPS(ISYS) would then be set equal to 0.75.

H5. Point Source Loading Segments and Point Source Loads

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	15		70	75
BPS(1,ISYS)	IPS(1,ISYS)	. . .	BPS(NOPS,ISYS)	IPS(NOPS,ISYS)

FORMAT(5(F10.0,I5)

BPS(I,ISYS) = point source load (kg/day)
IPS(I,ISYS) = index number of the point source load

Time-Variable Conditions (IPSOPT = 2)

H3. Time of Point Source Loading Specifications

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

20	30
NXPSTSECS	TWARPPS

FORMAT (10X, I10,6X,A4)

NXPSTSECS = time in seconds (or units specified by TWARPPS
TWARPPS = units to be used for NXPSTSECS
- = SECS or secs,
- = MINS or mins,
- = HRS or hrs,
- = DAYS or days.

Data associated with Data Types H4 through H7 will be read NOSYS times; once for each system in the model.

H4. Number of Point Source Loads

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NOPS(ISYS)

FORMAT(I10)

NOPS(ISYS) = the number of point source loads for system ISYS

(Note: if NOPS equal zero, then skip H5, H6 and H7 and continue with next H4 input.)

H5. Point Source Loads Scale Factor

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALPS(ISYS)

FORMAT(F10.0)

SCALPS(ISYS) = scale factor for system ISYS

H6. Point Source Loading Segments

20	30	40		80
IPS(1,ISYS)	IPS(2,ISYS)	IPS(3,ISYS)	- - -	IPS(NOPS,ISYS)

FORMAT(10X,7I10)

IPS(I,ISYS) = index number of the point source load

H7. Point Source Loads

20	30		80
BPS(1,ISYS)	BPS(2,ISYS)	- - -	BPS(NOPS(ISYS),ISYS)

FORMAT(10X,7F10.0)

BPS(I,ISYS) = point source loads (kg/day)

After input types H4 through H7 are repeated for each system, then the time of the next set of point source loads, NXPST, will be required; followed by the next set of point source loads (input type H7); it is not necessary to repeat input types H4, H5 and H6. If NOPS (ISYS) = 0 for system ISYS then no input type H7 is required either.

Table 7 presents an example input file for constant loading point source inputs. The user is referred back to Table 6 under GROUP G for an example of what a time-variable point source input file would look like.

TABLE 7. EXAMPLE OF TIME-INVARIANT OR CONSTANT POINT SOURCE INPUT - PSFILNA

```
C   IPSOPT
         1
C  NO   IX   IY Location / Vertical Distribution Fractions   (Index of Point Source Loads)
    1    5   16 Blue Plains WWTP
Fractions 0.25 0.25 0.25 0.25   0.   0.   0.   0.   0.   0.
    2   16    4 Deer Island WWTP
          0.25 0.25 0.25 0.25   0.   0.   0.   0.   0.   0.
    3   16    5 Nut Island WWTP
           0.5  0.5   0.   0.   0.   0.   0.   0.   0.   0.
    4   11   28 Tallman Island
           0.1  0.1  0.1  0.1  0.1  0.1 0 .1  0.1  0.1  0.1
    5    3   17 Rye Brook WWTP
            0.   0.   0.   0.   0.   0.   0.   0.  0.5  0.5
  -99           End of Point Source Loading Table Index
C  NOPS(1) - no point source loads for system 1
         0
C  NOPS(2) - number of loads for system 2
         5
C SCALPS(2) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
      250.   1       78.   2       6.3   4       25.   4       43.   5
C  NOPS(3) - number of loads for system 3
         5
C SCALPS(3) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
      240.   1       75.   2       6.0   4       22.   4       40.   5
C  NOPS(4) - number of loads for system 4
         5
C SCALPS(4) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
       24.   1       10.   2       0.7   4        2.   4        4.   5
C  NOPS(5) - number of loads for system 5
         4
C SCALPS(5) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
       24.   1       10.   2        2.   4        4.   5
C  NOPS(6) - number of loads for system 6
         5
C SCALPS(6) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
      2200.   1    1010.   2      250.   4      825.   4      460.   5
C  NOPS(7) - number of loads for system 7
         5
C SCALPS(7) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
      224.   1      110.   2      10.7   4       92.   4       74.   5
C  NOPS(8) - number of loads for system 8
         5
C SCALPS(8) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
      114.   1      310.   2       17.   4       52.   4       66.   5
C  NOPS(9) - number of loads for system 9
         5
C SCALPS(9) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
       44.   1       20.   2        8.   4       33.   4       24.   5
C NOPS(10) - number of loads for system 10
         5
C SCALPS(10) - scale factor
       1.0
C     Load IPS      Load IPS      Load IPS      Load IPS      Load IPS
      774.   1      510.   2       16.   4       89.   4       27.   5
```

GROUP I: NONPOINT SOURCE LOADS (NPSFILNA)

Inputs required for this group include:

1. nonpoint source loads input option
2. index table of nonpoint source loads
3. number of nonpoint source loads
4. scale factor for nonpoint source loads
5. actual nonpoint source loads

I1. <u>Nonpoint Source Loads Input Option</u>

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20
INPSOPT	INPSPWLOPT

FORMAT (2I10)

INPSOPT = input option
= 1, all nonpoint source loads are constant in time
= 2, time-variable nonpoint source loads will be used
INPSPWLOPT = option to select step-function or piecewise linear interpolation of time variable nonpoint source loadings
= 0, step function interpolation will be used,
= 1, piecewise linear interpolation will be used

The remaining nonpoint source loading inputs are dependent upon the INPSOPT input option chosen. Data inputs for option 1 (constant loads) will be presented first, followed by data inputs associated with option 2 (time-variable).

I2. <u>Index Table of Nonpoint Source Loads</u>

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5	10	15	65
INPS(1,I,ISYS)	INPS(2,I,ISY)	INPS(3,I,ISYS)	LOCATION

FORMAT (3I5,A50)

INPS(1,I,ISYS) = load identifier (should be numbered consecutively from 1 through the number of nonpoint source loads included in the model
= -99 to signal end of input
INPS(2,I,ISYS) = the x-cell number of the nonpoint source load
INPS(3,I,ISYS) = the y-cell number of the nonpoint source load.
LOCATION = a 50-character alpha-numeric description of the nonpoint source load locations, ex. 57th Street CSO

16	22	70
ZFRACNPS(1,I)	ZFRACNPS(2,I) . . .	ZFRACNPS(NZ,I)

FORMAT (10X,10F6.3)

ZFRACNPS(1,I) = fraction of point source load discharged to layer 1,2, . . ., through NZ (note: fractions should sum up to 1.0)
:
ZFRACPS(NZ,I) If a user wished to distribute a load equally throughout the water column and if NZ=10, then ZFRACNPS(1,I) through ZFRACNPS(10,I) would each be set to 0.1. If a user wished to put a load in the bottom two cells only (and again if NZ=10), then ZFRACNPS(1,I) through ZFRACNPS(8,I) = 0.0, and ZFRACNPS(9,I) = ZFRACNPS(10,I) = 0.5

Constant or Time-Invariant Loads (INPSOPT = 1)

Data associated with Data Types I3, I4 and I5 will be read NOSYS times; once for each system in the model.

I3. Number of Nonpoint Source Loads

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NONPS(ISYS)

FORMAT(I10)

NONPS(ISYS) = the number of nonpoint source loads for system ISYS

(Note: If there are no non-point source loads to be specified for a system (NONPS = 0), then no input is required for I4 or I5; just continue with next I3.

I4. Nonpoint Source Load Scale Factor

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALNPS(ISYS)

FORMAT(F10.0)

SCALNPS(ISYS) = scale factor for system ISYS

Normally SCALNPS(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in nonpoint source inputs, SCALNPS(ISYS) would then be set equal to 0.75.

I5. Nonpoint Source Loading Segments and Nonpoint Source Loads

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	15		70	75
BNPS(1,ISYS)	INPS(1,ISYS)	- - -	BNPS(NONPS,ISYS)	INPS(NONPS,ISYS)

FORMAT(5(F10.0,I5)

BNPS(I,ISYS) = nonpoint source load (kg/day)
INPS(I,ISYS) = index number of the nonpoint source load

Time-Variable Conditions (INPSOPT = 2)

I3. Time of Nonpoint Source Loading Specifications

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

20	30
NXNPSTSECS	TWARPNPS

FORMAT (10X, I10,6X,A4)

NXNPSTSECS = time in seconds (or units specified by TWARPNPS)
TWARPNPS = units to be used for NXNPSTSECS
= SECS or secs,
= MINS or mins,
= HRS or hrs,
= DAYS or days.

Data associated with Data Types I4 through I7 will be read NOSYS times; once for each system in the model.

I4. Number of Nonpoint Source Loads

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NONPS(ISYS)

FORMAT(I10)

NONPS(ISYS) = the number of nonpoint source loads for system ISYS

(Note: if NONPS equal zero, then skip I5, I6 and I7 and continue with next I4 input.)

I5. Nonpoint Source Loads Scale Factor

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALNPS(ISYS)
FORMAT(F10.0)

SCALNPS(ISYS) = scale factor for system ISYS

I6. Nonpoint Source Loading Segments

20 30 40 80
INPS(1,ISYS) INPS(2,ISYS) INPS(3,ISYS) - - - INPS(NONPS,ISYS
FORMAT(10X,7I10)

INPS(I,ISYS) = index number of the nonpoint source load grid element

I6. Nonpoint Source Loads

20 30 80
BNPS(1,ISYS) BNPS(2,ISYS) - - - BNPS(NONPS,ISYS)
FORMAT(10X,7F10.0)

BNPS(I,ISYS) = nonpoint source loads (kg/day)

After input types I4 through I7 are repeated for each system, then the time of the next set of nonpoint source loads, NXNPST, will be required; followed by the next set of nonpoint source loads (input type I7); it is not necessary to repeat input types I4, I5 and I6. If NONPS (ISYS) = 0 for system ISYS then no input type I7 is required either.

The user is referred back to Tables 6 and 7 for examples of what time-variable and constant input files would look like.

GROUP J: FALL-LINE LOADS
(FLFILNA)

Inputs required for this group include:

1. fall-line loads input option
2. index table of fall-line loads
3. number of fall-line loads
4. scale factor for fall-line loads
5. actual fall-line loads

J1. Fall-line Loads Input Option

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
IFLOPT IFLPWLOPT
FORMAT(2I10)

IFLOPT = input option
= 1, all fall-line loads are constant in time
= 2, time-variable fall-line loads will be used

IFLPWLOPT = option to select step-function or piecewise linear interpolation of time-variable fall-line source loadings.
= 0, step function interpolation will be used,
= 1, piecewise linear interpolation will be used.

The remaining fall-line loading inputs are dependent upon the IFLOPT input option chosen. Data inputs for option 1 (constant loads) will be presented first, followed by data inputs associated with option 2 (time-variable).

J2. Index Table of Fall-Line Loads

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

5	10	15	65
IFL(1,I,ISYS)	IFL(2,I,ISY)	IFL(3,I,ISYS)	LOCATION

FORMAT (3I5,A50)

IFL(1,I,ISYS) = load identifier (should be numbered consecutively from 1 through the number of fall-line loads included in the model
= -99 to signal end of input

IFL(2,I,ISYS) = the x-cell number of the fall-line load

IFL(3,I,ISYS) = the y-cell number of the fall-line load.

LOCATION = a 50-character alpha-numeric description of the fall-line load locations, ex. Branch Brook Inflow

16	22		70
ZFRACFL(1,I)	ZFRACFL(2,I)	. . .	ZFRACFL(NZ,I)

FORMAT (10X,10F6.3)

ZFRACFL(1,I)
:
ZFRACFL(NZ,I) = fraction of fall-line load discharged to layer 1,2, . . . , through NZ (note: fractions should sum up to 1.0) If a user wished to distribute a load equally throughout the water column and if NZ=10, then ZFRACFL(1,I) through ZFRACFL(10,I) would each be set to 0.1. If a user wished to put a load in the bottom two cells only (and again if NZ=10), then ZFRACFL(1,I) through ZFRACFL(8,I) = 0.0, and ZFRACFL(9,I) = ZFRACFL(10,I) = 0.5

<u>Constant or Time-Invariant Loads (IFLOPT = 1)</u>

Data associated with Data Types J3, J4 and J5 will be read NOSYS times; once for each system in the model.

J3. <u>Number of Fall-line Loads</u>

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5
NOFL(ISYS)

FORMAT(10)

NOFL(ISYS) = the number of fall-line loads for system ISYS

(Note: If there are no fall-line loads to be specified for a system (NOFL = 0), then no input is required for J4 or J5; just continue with next J3.)

J4. Fall-line Load Scale Factor

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALFL(ISYS)

FORMAT(F10.0)

SCALFL(ISYS) = scale factor for system ISYS

Normally SCALFL(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in fall-line inputs, SCALFL(ISYS) would then be set equal to 0.75.

J5. Fall-line Loading Segments and Fall-line Loads

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	15	70	75
BFL(1,ISYS)	IFL(1,ISYS)	BFL(NOFL,ISYS)	IFL(NOFL,ISYS)

FORMAT(5(F10.0,I5))

BFL(I,ISYS) = fall-line load (kg/day)
IFL(I,ISYS) = index number of the fall-line load

Time-Variable Conditions (IFLOPT = 2)

J3. Time of Fall-line Loading Specifications

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

20	30
NXFLTSECS	TWARPFL

FORMAT (10X, I10,6X,A4)

NXFLTSECS = time in seconds (or units specified by TWARPFL)
TWARPFL = units to be used for NXFLTSECS
= SECS or secs,
= MINS or mins,
= HRS or hrs,
= DAYS or days.

Data associated with Data Types J4 through J7 will be read NOSYS times; once for each system in the model.

J4. Number of Fall-line Loads

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5
NOFL(ISYS)

FORMAT(10)

NOFL(ISYS) = the number of fall-line loads for system ISYS

(Note: if NOFL equal zero, then skip J5, J6 and J7 and continue with next J4 input.)

J5. Fall-line Loads Scale Factor

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALFL(ISYS)

FORMAT(F10.0)

SCALFL(ISYS) = scale factor system ISYS

J6. Fall-line Loading Segments

20	30	40		80
IFL(1,ISYS)	IFL(2,ISYS)	IFL(3,ISYS)	- - -	IFL(NOFL,ISYS)

FORMAT(10X,7I10)

IFL(1,I,ISYS) = index number of the fall-line load

J7. Fall-line Loads

20	30		80
BFL(1,ISYS)	BFL(2,ISYS)	- - -	BFL(NOFL(ISYS),ISYS)

FORMAT(10X,7F10.0)

BFL(I,ISYS) = fall-line loads (kg/day)

After input types J4 through J7 are repeated for each system, then the time of the next set of fall-line loads, NXFLT, will be required; followed by the next set of fall-line loads (input type J7); it is not necessary to repeat input types J4, J5 and J6. If NOFL (ISYS) = 0 for system ISYS then no input type J7 is required either.

The user is referred back to Tables 6 and 7 for examples of what time-variable and constant input files would look like.

GROUP K: ATMOSPHERIC LOADS
(ATMFILNA)

Inputs required for this group include:

1. atmospheric loads input option
2. number of atmospheric loads
3. scale factor for atmospheric loads
4. actual atmospheric loads

K1. Atmospheric Loads Input Option

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20
IATMOPT	IATMPWLOPT

FORMAT (2I10)

IATMOPT = input option
= 1, all atmospheric loads are constant in time
= 2, time-variable atmospheric loads will be used
IATMPWLOPT = option to select step-function or piecewise linear interpolation of time-variable atmospheric loadings.
= 0, step-function interpolation will be used,
= 1, piecewise linear interpolation will be used.

The remaining atmospheric loading inputs are dependent upon the IATMOPT input option chosen. Data inputs for option 1 (constant loads) will be presented first, followed by data inputs associated with option 2 (time-variable).

Constant or Time-Invariant Loads (IATMOPT = 1)

Data associated with Data Types K2, K3 and K4 will be read NOSYS times; once for each system in the model.

K2. Number of Atmospheric Loads

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5
NOATM(ISYS)
FORMAT(I10)

NOATM(ISYS) = the number of atmospheric loads for system ISYS
= 0, no atmospheric loading for system ISYS
= 1, spatially-constant atmospheric loadings to water surface
= 2, spatially-variable atmospheric loadings to water surface

(Note: If there are no atmospheric inputs to be specified for a system (NOATM = 0), then no input is required for K3 or K4; just continue with next K2.

K3. Atmospheric Load Scale Factor

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALATM(ISYS)
FORMAT(F10.0)

SCALATM(ISYS) = scale factor for system ISYS

Normally SCALATM(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in atmospheric inputs, SCALATM(ISYS) would then be set equal to 0.75.

Spatially Constant Atmospheric Loads (NOATM (ISYS=1)

K4. Atmospheric Loading Rate

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

20
BATM(ISYS)

FORMAT(10X,F10.0)

BATM(ISYS) = atmospheric loading rate (kg/m^2-day)

RCA will take the areal atmospheric loading rate for system ISYS and apply this loading rate to each water segment in the model by multiplying the wetted surface area of the segment by the areal loading rate to compute the total kg/day loading to the water segment.

Spatially-Variable Atmospheric Loads (NOATM = 2)

K4. Atmospheric Loading Rates

20	30		80
BATM(1,1,ISYS)	BATM(2,1,ISYS)	- - -	BATM(NX,1,ISYS)
.	.		.
.	.		.
.	.		.

20	30		80
BATM(1,NY,ISYS)	BATM(2,NY,ISYS)	- - -	BATM(NX,NY,ISYS)

FORMAT(10X,7F10.0)

BATM(IX,IY,ISYS) = atmospheric loading rate (kg/m^2-day) for segment or grid cell (IX,IY) for system ISYS

Time-Variable Conditions (IATMOPT = 2)

K2. Time of Atmospheric Loading Specifications

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

20	30
NXATMTSECS	TWARPATM

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

NXATMTSECS = time in seconds (or units specified by TWARPATM
TWARPATM = units to be used for NXATMTSECS
= SECS or secs,

= MINS or mins,
= HRS or hrs,
= DAYS or days.

Data associated with Data Types K3, K4 and K5 will be read NOSYS times; once for each system in the model.

K3. Number of Atmospheric Loads

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

5
NOATM(ISYS)
FORMAT(10)

NOATM(ISYS) = the number of atmospheric loads for system ISYS
= 0, for no atmospheric loading for system ISYS
= 1, spatially-constant atmospheric loading to water surface

= 2, spatially-variable atmospheric loadings to water surface
(Note: if NOATM equal zero, then skip K4 and K5 and continue with next K3 input.)

K4. Atmospheric Loads Scale Factor

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALATM(ISYS)
FORMAT(F10.0)

SCALATM(ISYS) = scale factor for system ISYS

Spatially-Constant Atmospheric Loading (NOATM(ISYS) = 1)

K5. Atmospheric Loading Rate

```
              80
_________________
         Comment
_________________
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
          20
____________
BATM(ISYS)
FORMAT(10X,F10.0)
```

BATM(ISYS) = atmospheric loading rate (kg/m2-day)

Spatially-Variable Atmospheric Loads (NOATM(ISYS) = 2)

```
              80
_________________
         Comment
_________________
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

K5. Atmospheric Loading Rates

```
               20                 30                  80
BATM(1,1,ISYS)     BATM(2,1,ISYS)  - - - BATM(NX,1,ISYS)
        .                  .                  .
        .                  .                  .
        .                  .                  .

               20                 30                  80
BATM(1,NY,ISYS)   BATM(2,NY,ISYS) - - - BATM(NX,NY,ISYS)
FORMAT(10X,7F10.0)
```

BATM(IX,IY,ISYS) = atmospheric loading rate for segment or grid cell (IX,IY) for system ISYS

After input types K3 through K5 are repeated for each system, then the time of the next set of atmospheric loads, NXATMT, will be required; followed by the next set of atmospheric loads (input type K5); it is not necessary to repeat input types K3 and K4. If NOATM (ISYS) = 0 for a system then no input type K5 is required either.

RCA will take the areal atmospheric loading rate for system ISYS and apply it to each water segment in the model by and multiplying the wetted surface area of the receiving water segment by the loading rate to compute the total kg/day loading to the segment.

Tables 8 and 9 provide example input files for constant and time-variable inputs.

TABLE 8. EXAMPLE OF TIME-INVARIANT OR CONSTANT POINT SOURCE INPUT - PSFILNA

```
C  IATMOPT
         1
C  NOATM(1)   no salinity loads
         0
C  NOATM(2)   no phytoplankton loads
         0
C  NOATM(3)   no phytoplankton loads
         0
C  NOATM(4)   no RPOP loads
         0
C  NOATM(5)   no LPOP loads
         0
C  NOATM(6)   no RDOP loads
         0
C  NOATM(7)   no LDOP loads
         0
C  NOATM(8)   DPO4 load
         1
C  SCALATM
       1.0
C   PO4 load (kg/m2-day) == 0.011 mg P/L * 47 inches rainfall/yr
          0.3600E-07
C  NOATM(9)   no RPON loads
         0
C NOATM(10)   no LPON loads
         0
C NOATM(11)   no RDON loads
         0
C NOATM(12)   no LDON loads
         0
C NOATM(13)   NH4 loads
         1
C  SCALATM
       1.0
C  NH4 load (kg/m2-day) == 0.15 mg N/L * 47 in/yr = 0.15 g N/m3 * 1.194 m/yr * yr/365 day *
kg/1000 g
          0.4907E-06
C NOATM(14)   NO3 loads
         1
C  SCALATM
       1.0
C  NO3 load (kg/m2-day) == 0.43 mg N/L * 47 in/yr
          1.4066E-06
C NOATM(15)   no BSi loads
         0
C NOATM(16)   no DSI loads
  loads          0
C NOATM(17)   no RPOC loads
         0
C NOATM(18)   no LPOC loads
         0
C NOATM(19)   no RDOC loads
         0
C NOATM(20)   no LDOC loads
         0
C NOATM(21)   no ReDOC loads
         0
C NOATM(22)   no ExDOC loads
         0
C NOATM(23)   no O2eq loads
         0
C NOATM(24)   no DO loads
          0
```

TABLE 9. EXAMPLE OF TIME-VARIABLE ATMOSPHERIC INPUT - ATMFILNA TABLE

```
C  IATMOPT IATMPWLOPT
         2         0
          NXATMTSECS  TWARPATM
                    0      DAYS
C  NOATM(1)   no salinity load
         0
C  NOATM(2)   no phytoplankton load
         0
C  NOATM(3)   no phytoplankton load
         0
C  NOATM(4)   no RPOP load
         0
C  NOATM(5)   no LPOP load
         0
C  NOATM(6)   no RDOP load
         0
C  NOATM(7)   no LDOP load
         0
C  NOATM(8)   DPO4 load
         1
C  SCALATM        assumes 0.011 mg P/L in rainfall and the value specified by BATM is
 2.794E-06        monthly-averaged rainfall in inches/day
C   PO4 load      following value is total rainfall in January (3.1 inches) / 31 days
               0.100
C  NOATM(9)   no RPON load
         0
C NOATM(10)   no LPON load
         0
C NOATM(11)   no RDON load
         0
C NOATM(12)   no LDON load
         0
C NOATM(13)   NH4 load
         1
C  SCALATM        assumes 0.15 mg N/L in rainfall and the value specified by BATM is
 3.810E-05        monthly-averaged rainfall in inches/day
C  NH4 load       following value is total rainfall in January (3.1 inches) / 31 days
               0.100
C NOATM(14)   NO3 load
         1
C  SCALATM        assumes 0.43 mg N/L in rainfall and the value specified by BATM is
 1.092E-04        monthly-averaged rainfall in inches/day
C  NO3 load       following value is total rainfall in January (3.1 inches) / 31 days
               0.100
C NOATM(15)   no BSi load
         0
C NOATM(16)   no DSI load
         0
C NOATM(17)   no RPOC load
         0
C NOATM(18)   no LPOC load
         0
C NOATM(19)   no RDOC load
         0
C NOATM(20)   no LDOC load
         0
C NOATM(21)   no ReDOC load
         0
C NOATM(22)   no ExDOC load
         0
C NOATM(23)   no O2eq load
         0
C NOATM(24)   no DO load
         0
TIME              31
 PO4         0.07786      2.18 inches / 28 days
 NH4         0.07786      2.18 inches / 28 days
 NO3         0.07786      2.18 inches / 28 days
TIME              59
 PO4         0.10581      3.28 inches / 31 days
 NH4         0.10581      3.28 inches / 31 days
 NO3         0.10581      3.28 inches / 31 days
TIME              90
 PO4         0.08500      2.55 inches / 30 days
 NH4         0.08500      2.55 inches / 30 days
 NO3         0.08500      2.55 inches / 30 days
TIME             120
 PO4         0.08903      2.76 inches / 31 days
```

TABLE 9. EXAMPLE OF TIME-VARIABLE ATMOSPHERIC INPUT - ATMFILNA TABLE (Cont.)

```
 NH4         0.08903      2.76 inches / 31 days
 NO3         0.08903      2.76 inches / 31 days
TIME             151
 PO4         0.01060      3.18 inches / 30 days
 NH4         0.01060      3.18 inches / 30 days
 NO3         0.01060      3.18 inches / 30 days
TIME             181
 PO4         0.04871      1.51 inches / 31 days
 NH4         0.04871      1.51 inches / 31 days
 NO3         0.04871      1.51 inches / 31 days
TIME             212
 PO4         0.03581      1.11 inches / 31 days
 NH4         0.03581      1.11 inches / 31 days
 NO3         0.03581      1.11 inches / 31 days
TIME             243
 PO4         0.13500      4.05 inches / 30 days
 NH4         0.13500      4.05 inches / 30 days
 NO3         0.13500      4.05 inches / 30 days
TIME             273
 PO4         0.06484      2.01 inches / 31 days
 NH4         0.06484      2.01 inches / 31 days
 NO3         0.06484      2.01 inches / 31 days
TIME             304
 PO4         0.08266      2.48 inches / 30 days
 NH4         0.08266      2.48 inches / 30 days
 NO3         0.08266      2.48 inches / 30 days
TIME             334
 PO4         0.05677      1.76 inches / 31 days
 NH4         0.05677      1.76 inches / 31 days
 NO3         0.05677      1.76 inches / 31 days
TIME             366
```

GROUP L: PARAMETERS, CONSTANTS AND TIME-VARIABLE FUNCTIONS (PCFILNA)

Inputs required for this group include:

1. number of 2-D parameters
2. scale factors for 2-D parameters
3. parameter names
4. actual 2-D parameters
5. number of 3-D parameters
6. scale factors for 3-D parameters
7. parameter names
8. actual 3-D parameters
9. number of constants
10. actual constants
11. number of time-variable functions (tvfs)
12. tvf name and the number of time-breaks required to specify the tvf
13. actual tvfs
14. number of kinetic specific input file names
15. file names

L1. The Number of 2-Dimensional Parameters

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5
NPARM2D

FORMAT(10)

NPARM2D = number of 2-dimensional (or depth-independent) parameters

If there are no 2-D parameters to be read, skip over the next three input types and proceed with input type L5.

L2. 2-D Scale Factors

```
            80
       Comment
FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
       10         20                       80
PSCAL(1)  PSCAL(2)  - - -  PSCAL(NPARM2D)
FORMAT(8F10.0)
```

PSCAL(I) = scale factor for the Ith 2-D parameter set

L3. Parameter Name

```
     20
PNAME
FORMAT(A20)
```

PNAME = alphanumeric name for parameter set to be read

L4. 2-D Parameters

```
             10               20               30                         80
PARAM2D(1,1,I)  PARAM2D(2,1,I)  PARAM2D(3,1,I)  - - -  PARAM2D(NX1,2,I)
        .          .                    .                       .
        .          .                    .                       .
        .          .                    .                       .
              10                 20                    80
PARAM2D(1,NY,I)  PARAM2D(2,NY,I)  - - -  PARAM2D(NX,NY,I)
FORMAT(8F10.0)
```

PARAM2D(IX,IY,I) = value of the Ith parameter in segment or grid cell (IX,IY)

The parameters for the Ith parameter set are read a column at a time. The equivalent FORTRAN read statements would be:

```
DO I = 1,NPARM2D
 DO IY = 1,NY
  READ *, (PARAM2D(IX,IY,I), IX = 1, NX)
 ENDDO
ENDDO
```

L5. The Number of 3-Dimensional Parameters

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

5
NPARM3D

FORMAT(10)

NPARM3D = number of 3-dimensional (or depth-dependent) parameters

If there are no 3-D parameters to be read, skip over the next three input types and proceed with input type L9.

L6. 3-D Parameter Scale Factors

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20		80
PSCAL(1)	PSCAL(2)	- - -	PSCAL(NPARM3D)

FORMAT(8F10.0)

PSCAL(I) = scale factor for the Ith 3-D parameter set

L7. Parameter Name

20
PNAME

FORMAT(A20)

PNAME = alphanumeric name for parameter set to be read

L8. 3-D Parameters

```
                10                20                        80
PARAM3D(1,1,1,I)  PARAM3D(2,1,1,I)  - - -  PARAM3D(NX,1,1,I)
        .                .                          .
        .                .                          .
        .                .                          .
                   10                                    80
PARAM3D(1,NY,NZ,I)          - - -           PARAM3D(NX,NY,NZ,I)
FORMAT(8F10.0)
```

PARAM3D(IX,IY,IZ,I) = value of the Ith parameter in segment (IX,IY,IZ)

The parameters for the Ith parameter set are read by layer, by column. The equivalent FORTRAN read statement would be:

```
DO I = 1,NPARM3D
 DO IZ = 1,NZ
  DO IY = 1,NY
   READ *,(PARAM3D(IX,IY,IZ,I), IX = 1, NX)
  ENDDO
 ENDDO
ENDDO
```

Input types L7 and L8 are read for each parameter set, from 1 through NPARM3D.

L9. Number of Constants

```
            80
       Comment
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
    5
NCONS
FORMAT(10)
```

NCONS = number of constants to be read

If no constants are to be read, set NCONS equal to 0 and continue with input type L11.

L10. Constants

```
        10          20              80
CNAME(1)  CNAME(2)  - - -  CNAME(8)
CONST(1)   CONST(2)  - - -  CONST(8)
        .           .               .
        .           .               .
        .           .               .
CNAME(NOCONS-1) CNAME(NOCONS)
CONST (NOCONS-1) CONST (NOCONS)
FORMAT(8A10/8F10.0)
```

CNAME(1) = name of the Ith constant
CONST(I) = value of the Ith constant

The specification of CNAME is optional, but by specifying alphanumeric text it facilitates editing the constants section of the input file.

L11. Number of Time-Variable Functions (TVFs)

```
             80
        Comment
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
        5          10
NOFUNC  ITVFPLOPT
FORMAT(210)
```

NOFUNC = number of time-variable functions to be read
ITVFPLOPT = step function or piecewise linear interpolation option
= 0, use step function
= 1, use piece wise linear interpolation

Data associated with Data Types L12 and L13 will be read NOFUNC times; once for each time-variable function required by the model.

L12. TVF Name and the Number of TVF Time Breaks
(Note if NOFUNC = 0, no input is required for L12 and L13.)

```
             80
        Comment
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

5	10	20
PNAME	NOBRK	TWARPTWF

FORMAT
(A10,10,6X,A4)

PNAME = name of the time-variable function (tvf)
NOBRK = number of time breaks required to specify the tvf
TWARPTWF = units to be used for the time breaks in the tvf.
= SECS or secs,
= MINS or mins,
= HRS or hrs,
= DAYS or days.

L13. Time-Variable Function

10	20	30	40		70	80
VALT(1)	T(1)	VALT(2)	T(2)	- - -	VALT(NOBRK)	T(NOBRK)

FORMAT(8F10.0)

VALT(I) = value of the function at time T(I)
T(I) = time in seconds (or units specified by TWARPTVF).

Note: Unlike previous versions of RCA all tvfs do not have to use the same time breaks (T(I)).

L14. Number of Miscellaneous Input Files to be Used by the Kinetic Subroutine

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
NOKINFILNA

FORMAT (I10)

NOKINFILNA = number of file names to be read

L15. File Names

40
KINFILNA(I)
FORMAT(A40)

KINFILNA(I) = complete path length and file name for kinetic subroutine input file I. The number of file names and the order in which they are specified is determined by the kinetic subroutine being used.

Table 10 presents a sample parameter, constant, tvf input file for a model with 10 cells in the x-direction, 5 cells in the y-direction, and 2 vertical layers with two 2-D parameters, one 3-D parameter, 44 constants, 1 time-variable function and 2 kinetic subroutine specific input files.

TABLE 10. EXAMPLE OF A PARAMETER, CONSTANTS AND TIME-VARIABLE FUNCTION INPUT FILE - PCFILNA

```
C N2DPARAM
         2
C   Scale1    Scale2
    0.3048       1.0
C   Ke - extinction coefficient
     0.000     0.000     0.000     0.000     0.000     0.000     0.000     0.000
     0.000     0.000
     0.000     0.787     0.787     0.850     0.880     0.925     1.250     1.150
     1.050     0.000
     0.000     0.787     0.787     0.850     0.880     0.920     1.170     1.120
     1.000     0.000
     0.000     0.787     0.787     0.840     0.870     0.900     0.980     1.100
     1.000     0.000
     0.000     0.000     0.000     0.000     0.000     0.000     0.000     0.000
     0.000     0.000
C   Kl - mass trasnfer coefficient  (reaeration coefficient)
       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
       0.0       0.0
       0.0       1.5       1.5       1.5       1.5       1.0       1.0       1.0
       1.5       0.0
       0.0       1.5       1.5       1.5       1.5       1.0       1.0       1.0
       1.5       0.0
       0.0       1.5       1.5       1.5       1.5       1.0       1.0       1.0
       1.5       0.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
       0.0       0.0
C N3DPARAM
         1                                    number of 3D parameters
C    SCALE
   1.0E-00
C   SS (mg/L)
       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
       0.0       0.0                                    layer 1
       0.0       15.       15.       15.       14.       12.       10.       10.
       10.       0.0
       0.0       15.       15.       15.       14.       12.       10.       10.
       10.       0.0
       0.0       15.       15.       15.       14.       12.       10.       10.
       10.       0.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
       0.0       0.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
       0.0       0.0                                    layer 2
       0.0       18.       18.       18.       16.       14.       12.       11.
       11.       0.0
       0.0       18.       18.       18.       16.       14.       12.       11.
       11.       0.0
       0.0       18.       18.       18.       16.       14.       12.       11.
       11.       0.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
       0.0       0.0
C    NCONS
        20                                   number of constants
     AGOPT     KAOPT     KEOPT    Unused    Unused     TOPT1   K1BETA1   K2BETA2
        0.        1.        2.                          3.50      .004      .006
       K1C       K1T       IS1      KMN1      KMP1      KMS1      K1RB      K1RG
     2.500     1.068   150.000     0.010     0.001     0.020     0.075       0.0
      K1RT     K1GZC     K1GZT     CCHL1     CPR11     CPR12     CPR13     CNR11
     1.047     0.100      1.10      30.0      40.0       0.0       0.0     5.670
     CNR12     CNR13     CSR11     CSR12     CSR13     TOPT2   K2BETA1   K2BETA2
       0.0       0.0       5.0      10.0       0.0       22.      .004      .006
       K2C       K2T       IS2      KMN2      KMP2      KMS2      K2RB      K2RG
     2.400     1.068     350.0     0.010     0.001     0.002     0.075        0.
      K2RT     K2GZC     K2GRT     CCHL2
     1.047     0.120     1.100      80.0
C    NOTVF  TVPWLOPT
         1         1                          number of time functions
C    PNAME     NOBRK  TWARPTVF
      ITOT        13      DAYS       TOTAL DAILY RADIATION
      118.        0.      168.       11.      218.       59.      318.       90.
      418.      120.      468.      151.      518.      181.      468.      212.
      418.      243.      318.      273.      218.      304.      168.      335.
      118.      365.
C NOKINFILNA
         2
sed.inp
/users/potomac/vegm.inp
```

GROUP M: INITIAL CONDITIONS

Inputs required for this group include:

1. sigma level or standard level input option
2. initial conditions

M1. Option to Read Initial Conditions Using Sigma Levels or Standard Levels

```
             80
________________
        Comment
________________
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
     10
_________
  ICOPT
_________
 FORMAT(I0)
```

ICOPT = sigma-level or standard level input option
= 0, use sigma-level
= 1, use standard level

Sigma-Level Initial Conditions (ICOPT=0)

M2. Initial Conditions (or Initial Solution Estimates)

```
             80
________________
        Comment
________________
  FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
               20                 30                       80
______________________________________________________________
CARAY(1,1,1,ISYS)  CARAY(2,1,1,ISYS)  - - -  CARAY(NX,1,1,ISYS)
       .               .               .               .
       .               .               .               .
       .               .               .               .

                  20                                       80
______________________________________________________________
CARAY(1,NY,NZ,ISYS)          - - -          CARAY(NX,NY,NZ,ISYS)
FORMAT(10X,7F10.0)
```

CARAY(IX,IY,IZ,ISYS)= initial condition for segment grid cell (IX,IY,IZ) for system ISYS

The initial conditions are read by system, by layer, by y-direction. The equivalent read statement would be:

```
DO ISYS = 1,NOSYS
 DO IZ = 1,NZ
  DO IY = 1,NY
   READ *, (CARAY(IX,IY,IZ,ISYS), IX = 1,NX)
  ENDDO
 ENDDO
ENDDO
```

Standard Level Initial Conditions (ICOPT=1)

M2. Number of Standard Levels

```
               80
          Comment
 FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
     10
 NLVLS
FORMAT(I10)
```

NLVLS = number of standard levels at which initial conditions are defined

M3. Standard Level Depths

```
        10           20                  80
SLDEPTH(1)  SLDEPTH(2) . . . SLDEPTH(NLVLS)
```

SLDEPTH(1) = the depth in meters of the ITH standard level

M4. Initial Conditions at Standard Levels

```
            20             30                     80
CARAYSL(1,1,1)  CARAYSL(2,1,1)   . . .   CARAYSL(NX1,1)
       .        .                            .
       .        .                            .
       .        .                            .
                  20                              80
CARAYSL(1,NY,NLVLS)    . . .    CARAYSL(NX,NY,NLVLS)
FORMAT(10X,7F10.0)
```

CARAYSL(IX,IY,IZ) = initial condition at standard depth level IZ for segment grid cell (IX,IY)

APPENDIX A

INTEGRATED EUTROPHICATION AND SEDIMENT NUTRIENT FLUX MODELS

TABLE OF CONTENTS

TABLES

FIGURES

1.0 KINETIC FRAMEWORK FOR THE INTEGRATED EUTROPHICATION MODEL

1.1 INTRODUCTION

This portion of the RCA Users Guide describes an integrated eutrophication/sediment nutrient flux modeling framework, available with the Public Domain release of RCA. In addition, the range in kinetic coefficients used in a number of eutrophication studies performed by HydroQual are provided as a reference.

1.1.1 Conservation of Mass

The modeling framework described in this document is based upon the principle of conservation of mass. The conservation of mass accounts for all of a material entering or leaving a body of water, transport of the material within the water body, and physical, chemical and biological transformations of the material. For an infinitesimal volume oriented along the axis of a three-dimensional coordinate system, a mathematical formulation of the conservation of mass may be written:

$$\frac{\partial c}{\partial t} = \underbrace{\frac{\partial}{\partial x}\left(E_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \frac{\partial c}{\partial z}\right)}_{\text{dispersive transport}} \underbrace{- U_x \frac{\partial c}{\partial x} - U_y \frac{\partial c}{\partial y} - U_z \frac{\partial c}{\partial z}}_{\text{advective transport}} \tag{1-1}$$

$$\underbrace{\pm S(x,y,z,t)}_{\text{sources or sinks}} + \underbrace{W(x,y,z,t)}_{\text{external inputs}}$$

where:

c = concentration of the water quality variable [M/L^3],
t = time [T],
E = dispersion (mixing) coefficient due to tides and density and velocity gradients (L^2/T),
U = advective velocity (L/T),
S = sources and sinks of the water quality variable, representing kinetic interactions (M/L^3-T),
W = external inputs of the variable c (M/L^3-T),
x,y,z = longitudinal, lateral and vertical coordinates,
M,L,T = units of mass, length and time, respectively.

The modeling framework is made up of two components: (1) the transport due to freshwater flow in riverine systems and/or tidal, meteorological and density-driven currents in esturaine and coastal systems, and (2) the kinetic interactions between variables and the external inputs . Freshwater flow and/or density-driven currents and tidally and wind induced mixing are responsible for the movement of the water quality constituents within the waterbody.

External inputs of nutrients and oxygen-demanding material are derived from numerous sources, including: municipal and industrial discharges, combined sewer overflows (CSOs), storm sewer overflows (SSOs), natural surface runoff, and atmospheric deposition to the water surface of the waterbody.

The kinetics control the rates of interactions among the water quality constituents. Ideally, in a modeling effort, they should be independent of location per se, although they may be functions of exogenous variables, such as temperature and light, which may vary with location.

Analytical solutions are not available for partial differential equations of the form of Equation 1-1 except for the simplest cases. Instead, numerical methods are utilized to solve these mass balance equations. A specific method of solution employed in a majority of water quality modeling frameworks is known as the finite difference technique. First, the estuary is divided into finite volumes. Then a finite difference approximation of Equation 1-1 is applied to the ith finite volume or segment, resulting in an equation of the form (see Thomann and Mueller, 1987):

$$V_i \frac{dc_i}{dt} = \sum_{j=1}^{n} R_{ij}\left(c_j - c_i\right) + \sum_{k=1}^{n} Q_{ki} c_k - \sum_{m=1}^{n} Q_{im} c_i \pm S_i + W_i \qquad (1\text{-}2)$$

$$i = 1, 2, \ldots n \text{ (where } n = \text{number of segments)}$$

where

V_i = volume of segment i (L^3),
c_i = concentration of the water quality variable in the ith segment, (M/L^3),
R_{ij} = exchange between segment i and j resulting from dispersive mixing, (L^3/T),
Q_{ki} = net advective flow entering segment i from segment k, (L^3/T),
Q_{im} = net advective flow leaving segment i and going to segment m, (L^3/T),
S_i = sources and sinks, in segment i representing kinetic interactions, (M/T),
W_i = external inputs to segment i (M/T).

The exchange coefficients and advective flows are computed from

$$R_{ij} = \frac{E_{ij}\ A_{ij}}{L_{ij}} \qquad (1\text{-}3a)$$

and

$$Q_{ij} = A_{ij}\ U_{ij} \qquad (1\text{-}3b)$$

respectively, where E_{ij} is the dispersion coefficient, representing the overall phenomenon of mixing due to temporal variations in the tidal velocity, lateral and vertical gradients in velocity, and density differences within the water body; A_{ij} is the cross-sectional area of the ij interface; L_{ij} is the characteristic length defined as $(L_i + L_j)/2$; and U_{ij} is the net advective velocity from segment i to j. The term S_i, the sources and sinks of material in segment i, represents the kinetic interactions (physical, chemical and biological) occurring within the segment. These interactions may be functions only of the variable under consideration, for example, the first order decay of organic material. Alternately, they may involve the interactions between other variables, e.g., the first order feed-forward interaction between the oxidation of organic carbon (BOD) and dissolved oxygen, or the more complex interactions between phytoplankton biomass and nutrients, which involve non-linear feed-forward and feed-back interactions. The term W_i represents the external inputs of material into segment i, including point and nonpoint source loads, CSO loads, and/or atmospheric loads.

Mass balance equations in the form of Equation 1-2 are formulated for each segment in the estuary and for each state-variable included in the modeling framework. This results in *n x m* simultaneous finite difference equations to be solved, where *n* is the number of segments and *m* is the number of state-variables.

1.1.2 Choice of State Variables

An important criterion for the inclusion of variables in a modeling framework is the existence of adequate field data for calibration/verification of the variable, as well as the importance of the variable in the processes being considered. The kinetic framework employed of the integrated eutrophication is based on the LIS 3.0 eutrophication model developed for the Long Island Sound Study (HydroQual, Inc. 1991), the Massachusetts Bays Eutrophication Model (BEM) developed for the Massachusetts Water Resources Authority (MWRA) and the modeling effort of the Chesapeake Bay system (Cerco and Cole, 1995) and utilizes the following 26 state variables:

1. - salinity (S)
2. - phytoplankton carbon - winter assemblage (P_{c1})
3. - phytoplankton carbon - summer assemblage (P_{c2})
4. - phytoplankton carbon - fall assemblage (P_{c3})
5. - refractory particulate organic phosphorus (RPOP)
6. - labile particulate organic phosphorus (LPOP)
7. - refractory dissolved organic phosphorus (RDOP)
8. - labile dissolved organic phosphorus (LDOP)
9. - algal phosphorus + dissolved inorganic phosphorus (PO_4T)
10. - refractory particulate organic nitrogen (RPON)
11. - labile particulate organic nitrogen (LPON)
12. - refractory dissolved organic nitrogen (RDON)
13. - labile dissolved organic nitrogen (LDON)
14. - algal nitrogen + ammonia nitrogen (NH_4T)
15. - nitrite + nitrate nitrogen (NO_2+NO_3)
16. - biogenic silica - unavailable (SiU)
17. - algal silica + available silica (SiT)
18. - refractory particulate organic carbon (RPOC)
19. - labile particulate organic carbon (LPOC)
20. - refractory dissolved organic carbon (RDOC)
21. - labile dissolved organic carbon (LDOC)
22. - algal exudate dissolved organic carbon (ExDOC)
23. - reactive particulate organic carbon (RePOC)
24. - reactive dissolved organic carbon (ReDOC)
25. - dissolved oxygen equivalents (O_2^*)
26. - dissolved oxygen (DO)

The kinetic equations discussed below incorporate these state variables and are designed to simulate the annual cycle of phytoplankton production, its relation to the supply of nutrients and its effect on dissolved oxygen. The calculation is based on formulating the kinetics which govern the interactions of the biota and the various nutrient forms, and the application of these kinetics to the waterbody within the context of mass conservation equations.

1.2 MODEL KINETICS

1.2.1 General Structure

Salinity is included in the eutrophicaton modeling framework to enable verification that the transport structure of the hydrodynamic model (Blumberg and Mellor, 1987) is transferred to the water quality model properly. For salinity there are no reaction kinetics involved, i.e., they are conservative. There are no direct sources or sinks of salinity, other than via exchange with the model boundaries or via freshwater dilution resulting from wastewater treatment facility discharges, CSOs, etc. and from freshwater rivers draining into the waterbody.

Figure 1-1 presents the principal kinetic interactions for the nutrient cycles and dissolved oxygen. In the phosphorus system kinetics, dissolved inorganic phosphorus (DIP) is utilized by phytoplankton for growth. Phosphorus is returned from the phytoplankton biomass pool to the various dissolved and particulate organic phosphorus pools and to DIP through endogenous respiration and predatory grazing. The various forms of organic phosphorus are converted to DIP at a temperature dependent rate.

The kinetics of the nitrogen species are fundamentally the same as the kinetics of the phosphorus system. Ammonia and nitrite + nitrate are used by phytoplankton for growth. Ammonia is the preferred form of inorganic nitrogen for algal growth, but phytoplankton will utilize nitrite + nitrate nitrogen as ammonia concentrations become depleted. Nitrogen is returned from algal biomass and follows pathways that are similar to those of phosphorus. Organic nitrogen is converted to ammonia at a temperature dependent rate, and ammonia is then converted to nitrite + nitrate (nitrification) at a temperature and oxygen dependent rate. Nitrite + nitrate may be converted to nitrogen gas (denitrification) in the absence of oxygen at a temperature dependent rate.

Available silica is utilized by diatom phytoplankton during growth. Silica is returned to the unavailable silica pool during respiration and predation and must undergo mineralization processes before becoming available for phytoplankton growth.

Dissolved oxygen is coupled to the other state variables. The sources of oxygen considered are reaeration and algal photosynthesis. The sinks of oxygen are algal respiration, oxidation of detrital carbon and carbonaceous material from wastewater treatment plant effluents and nonpoint discharges, nitrification and SOD.

Organic carbon sources include anthropogenic inputs and the by-products of primary production and zooplankton grazing. The kinetic subroutine also incorporates two highly reactive organic carbon pools that can be used to represent organic carbon inputs from combined sewer overflows (CSOs) and/or waste water treatment plants (WWTPs) with poor treatment performance. The sink of organic carbon is via bacterial decomposition or oxidation. Specific details for the above reactions are presented below.

1.2.2 Phytoplankton Growth and Loss Kinetics

The current implementation of RCA permits the user to simulate up to three functional algal groups. They may represent a winter diatom group, a summer mixed assemblage, a fall mixed assemblage or they may represent a winter diatom group, a late spring/summer green group, and a late summer blue-green species (such as *Microcystis* or *Amabena*). The user, however, does have the option of implementing one, two, or three groups. In case, any kinetic framework employed for all three functional algal groups is the same, only the choice of model coefficients is different. It is convenient to express the kinetic source term for phytoplankton, S_P, as the difference between the phytoplankton growth rate, G_P, and the loss rate, D_P. That is:

$$S_p = (G_p - D_p)P \tag{1-4}$$

where P is the phytoplankton biomass (in units of carbon), and where G_P and D_P have units (day^{-1}). The balance between the magnitude of the growth rate and the loss rate (together with the transport and mixing) determines the rate at which phytoplankton mass is created (or lost) in each volume element.

The growth rate of a population of phytoplankton in a natural environment is a complicated function of the species of phytoplankton present and their differing reactions to solar radiation, temperature, and the balance between nutrient availability and nutrient requirements. In order to construct a growth function, a simplified approach is followed. Rather than consider the problem of different species and their associated environmental and nutrient requirements, the population is characterized as a whole by a measurement of the biomass of the phytoplankton present.

For single species, the direct measure of the population size is the number of cells per unit volume. Cell counts of a single species may be obtained fairly readily in a well-controlled laboratory environment. However, in naturally occurring populations, this measure may be somewhat ambiguous. It is often difficult to distinguish between viable and non-viable cells, and colonizing species tend to pose a problem because counts usually do not distinguish individual cells, and the sizes of the colonies are quite variable.

The sum of the numbers of each species, the total count, could be used to characterize biomass, but since cell size varies substantially, the pico-phytoplankton would dominate such an aggregation. To account for this, the total bio-volume, or wet weight of phytoplankton, assuming unit density, can be calculated using characteristic volumes for each identified species. Unfortunately, volumes can vary appreciably as a function of nutrient availability. Conversion to phytoplankton dry weight and carbon involves further species-dependent constants, which are also nutrient dependent, and, therefore, are subject to variation and uncertainty. Thus, although the use of phytoplankton dry weight or carbon concentration is an appealing solution to the issue of aggregation, it suffers from some practical difficulties.

An alternative approach to this problem is to measure a parameter which is characteristic of all phytoplankton, namely, chlorophyll-a (chl-a), and to use this as the aggregated variable. The principal advantages are that the measurement is direct, it integrates cell types and age, and it accounts for cell viability. The principal disadvantages are that it is a community measurement with no differentiation between functional groups (for example, diatoms or blue-green algae), and it is not necessarily a good measurement of standing crop in dry weight or carbon units, since the chlorophyll to dry weight and chlorophyll to carbon ratios are variable, and non-active chlorophyll (phaeo-pigments) must be measured to determine viable chlorophyll concentrations.

As can be seen from the above discussion, no simple aggregate measurement is entirely satisfactory. From a historical and practical point of view, the availability of extensive chlorophyll-a data for many waterbodies essentially dictates its use as the aggregate measure of the phytoplankton population, or biomass, for calibration and verification purposes. However, for internal computations, the eutrophication model uses phytoplankton carbon as a measure of algal biomass. The reasons for choosing phytoplankton carbon, rather than chl-a as the internal state variable, are twofold. The first reflects the fact that measures of primary production (an important measure of carbon fixation or growth) are made in carbon units. The second reason is that the use of phytoplankton carbon greatly facilitates the model computation of oxygen-demanding material deposited to the sediment bed via settling.

1.2.2.1 Standard Algal Growth Model

At the current time, HydroQual uses one of two algal growth model formulations. The first of these (to be referred to as the "standard" algal growth model formulation) dates back to the early work of DiToro, O'Connor, and Thomann on the Sacramento-San Joaquin River system (DiToro et al., 1971), the Great Lakes (DiToro and Matystik, 1980, DiToro and Connolly, 1980), and the Potomac Estuary (Thomann et al, 1974, Thomann and Fitzpatrick, 1982). The second algal growth model (to be referred to as the Laws and Chalup model) is based on the model developed by Laws and Chalup (1990) and applied by HydroQual (1995) to the Massachusetts Bays system.

To date, the standard model has been applied by HydroQual to more studies than has the Laws and Chalup model, but we feel there is merit in making both versions of the algal growth model available to the user. The details of the standard model will be presented first, followed by the Laws and Chalup model. These in turn will be followed by a description of the nutrient and dissolved oxygen kinetics.

With the choice of biomass units established, i.e., a carbon based system (mg C/L or gm C/m^3), a growth rate, which expresses the rate of production of biomass as a function of the important environmental variables, temperature, light and nutrients, may be developed. The specific growth rate, G_P, is related to G_{Pmax}, the maximum growth rate at optimum light, temperature and nutrients, via the following equation:

$$G_p = G_{P\max} \cdot \underset{\text{temperature}}{G_T(T)} \cdot \underset{\text{light}}{G_I(I)} \cdot \underset{\text{nutrients}}{G_N(N)} \tag{1-5}$$

where
$G_T(T)$ is the effect of temperature, $G_I(I)$ is the light attenuation given by

$$G_I(I) = g(I, f, H, k_e) \tag{1-6}$$

and $G_N(N)$ is the nutrient limitation given by

$$G_N(N) = g(DIP, DIN, Si) \tag{1-7}$$

where T is the ambient water temperature; I is the incident solar radiation; f is the fraction of daylight; H is the depth of the water column; k_e is the extinction or light attenuation coefficient; and DIP, DIN and Si are the available nutrients required for growth, dissolved inorganic phosphorus (ortho-phosphate), dissolved inorganic nitrogen (ammonia plus nitrite/nitrate) and dissolved available silica, respectively.

Initial estimates of G_{Pmax} are generally based upon the literature and/or previous modeling studies and are subsequently refined during the calibration process. During the simulation, the selected maximum growth rates are temperature corrected using spatially-dependent, time-dependent water column temperature values as computed by the hydrodynamic model. The temperature corrected growth rate is computed using one of the two following equations, which relates $G_{Pmax}(T)$, the growth rate at ambient temperature, T, to $G_{Pmax}(T_{20})$ the growth rate at 20°C (via equation (1-8a)) or to $G_{Pmax}(T_{opt})$, the growth rate at the optimal temperature, T_{opt} (via equations (1-8b) and (1-8c)):

$$G_{P\max}(T) = G_{P\max}(T_{20})\ \theta^{T-20} \tag{1-8a}$$

$$G_{P\max}(T) = G_{P\max}\, e^{-\beta_1 (T_{opt} - T)^2} \qquad T \le T_{opt} \tag{1-8b}$$

or

$$G_{P\max}(T) = G_{P\max}\, e^{-\beta_2 (T_{opt} - T)^2} \qquad T > T_{opt} \tag{1-8c}$$

where θ is the Arrenhius temperature coefficient, and β_1 and β_2 are shaping coefficients. When using equations 1-8b and 1-8c to temperature correct G_{Pmax}, T_{opt} has a much lower value for winter diatoms then would be used for the summer mixed assemblage. It is suggested to utilize the Arrenhius formulation when modeling one functional algal group and the shaped formulation when modeling two or more functional groups.

Figure 1-2 presents comparisons of the two temperature correction formulations. In Figure 1-2a, the normalized growth rates are compared for the Arrenhius (normalized to the 20°C growth rate versus the shaped formulation (normalized to the maximum growth rate at the optimum temperature) for a winter temperature optimum of 8°C and a summer temperature optimum of 24°C. Figure 1-2b presents a similar comparison but for "actual" growth rates of 1.7, 2.2, and 3.0 day for the Arrenhius, winter-shaped, and summer-shaped formulations. The temperature corrected growth rate is then adjusted to reflect effects due to ambient light and nutrient levels.

In the natural environment, the light intensity to which the phytoplankton are exposed is not uniformly at the optimum value. At the surface and near-surface of the air-water interface, photo-inhibition can occur due to high light intensities, while at depths below the euphotic zone, light is not available for photosynthesis due to natural and algal related turbidity. The light formulation included in the standard RCA modeling framework extends from a light curve analysis by Steele (1962) and accounts for both the effects of saturating light intensities and light attenuation through the water column. The depth-averaged light attenuated growth rate factor, $G_I(I)$, is presented in Equation 1-9 and is obtained by integrating the specific growth rate over depth:

where:

$$G_I(I) = \frac{e}{k_e H}\left[\exp\left(\frac{-I_o(t)}{I_s} e^{-k_e H}\right) - \exp\frac{-I_o(t)}{I_s}\right] \tag{1-9}$$

e = 2.718
H = the water column depth or thickness of the water cell or segment (m),
k_e = the total extinction coefficient, $k_{ebase} + k_c\, P_{chl\text{-}a}$ computed from the sum of the base, non-algal related, light attenuation, k_{ebase}, and the self-shading attenuation due to the ambient phytoplankton population $k_c P_{chl\text{-}a}$ (m^{-1}),
k_c = the algal related extinction coefficient per unit of chlorophyll (m^2/mg chl-a),
$P_{chl\text{-}a}$ = the ambient phytoplankton population as chlorophyll (mg chl-a/L), where $P_{chl\text{-}a} = P_c / a_{cchl}$
P_c = the ambient phytoplankton population as carbon (mg C/L),
a_{cchl} = the ratio of algal carbon to algal chlorophyll (mg C/mg chl-a),
I_o = the incident light intensity at the segment surface (ly/day),
I_s = the saturating light intensity (ly/day).

The value of I_o at the water surface, I_{surf}, may be evaluated at any time, t, within the day using the following formula:

$$I_{surf}(t) = \frac{I_{tot}}{0.635\, f} \sin\left[\frac{\pi(t_d - t_{sunrise})}{f}\right] \tag{1-10}$$

where

I_{tot} = total daily incident solar radiation (ly/day),
f = fraction of daylight (daylight hours/24),
t_d = time of day,
$t_{sunrise}$ = time of sunrise

To account for the effect of variations of available light as a function of depth, the light intensity, I_o (H), at any depth, H, is related to the incident surface intensity, I_{surf}, via the extinction coefficient, k_e through the formula

$$I_o(H) = I_{surf} \exp^{-k_e H} \tag{1-11}$$

The effects of various nutrient concentrations on the growth of phytoplankton have been investigated, and the results are quite complex. As a first approximation to the effect of nutrient concentration on the growth rate, it is assumed that the phytoplankton population in question follows Monod growth kinetics with respect to the important nutrients. That is, at an adequate level of nutrient concentration, the growth rate proceeds at the saturated rate for the ambient temperature and light conditions. However, at low nutrient concentration, the growth rate becomes linearly proportional to nutrient concentration. Thus, for a nutrient with concentration N_j in the j^{th} segment, the factor by which the saturated growth rate is reduced in the j^{th} segment is $N_j/(K_m + N_j)$. The constant, K_m, which is called the Michaelis or half-saturation constant, is the nutrient concentration at which the growth rate is half the saturated growth rate. Since there are three nutrients, nitrogen, phosphorus and silica, considered in this framework, the Michaelis-Menton expression is evaluated for each nutrient and the minimum value is chosen to reduce the saturated growth rate,

$$G_N(N) = \mathrm{Min}\left(\frac{DIN}{K_{mN} + DIN}, \frac{DIP}{K_{mP} + DIP}, \frac{Si}{K_{mSi} + Si}\right) \tag{1-12}$$

Numerous mechanisms have been proposed which contribute to the death rate of phytoplankton: endogenous respiration, grazing by herbivorous zooplankton, sinking or settling from the water column and parasitization (Fogg, 1965). The first three mechanisms have been included in previous models for phytoplankton dynamics and they have been shown to be of general importance. For this version of the integrated eutrophication model, only endogenous respiration and settling have been explicitly included in the modeling framework. The effect of zooplankton grazing is included indirectly using a first-order temperature corrected algal loss rate.

The endogenous respiration rate of phytoplankton is the rate at which the phytoplankton oxidize their organic carbon to carbon dioxide per unit weight of phytoplankton organic carbon. Respiration is the reverse of the photosynthesis process, and as such, contributes to the loss rate of the phytoplankton population. If the respiration rate of the phytoplankton, as a whole, is greater than the growth rate, there is a net loss of phytoplankton carbon or biomass. The endogenous respiration rate has been shown to be temperature dependent (Riley et al., 1949) and historically has been included in eutrophication models using Equation 1-13a,

$$k_{PR}(T) = k_{PR}(20^{\circ}C) \cdot \theta_{PR}^{(T-20)} \tag{1-13a}$$

where k_{PR} (20°C) is the endogenous respiration rate at 20°C, and $k_{PR}(T)$ is the temperature corrected rate. The units of k_{PR} are day^{-1}.

However, more recently the literature (Laws and Bannister, 1980, Laws and Chalup, 1991) suggests that algal respiration should be divided into two components - basal or resting respiration and respiratory losses associated with photosynthesis. This may be written mathematically as follows:

$$k_{PR}(T) = r_g G_P + r_b\, \theta_{PR}^{T-20} \tag{1-13b}$$

where r_g is the fraction of the algal growth (G_P) lost to the energy cost of photosynthesis and r_b is the basal respiration rate. Note, the user can select either form of the respiration rate equation when performing a simulation. If the user wishes to use the first formulation (equation 1-13a) then set r_g equal to zero and use an appropriate value for r_b (~0.1-0.3/day). If the user wises to use the latter form (equation 1-13b) then set r_g to a non-zero value (0.1-0.3) and use a lower value (0.01-0.03/day) for r_b.

The sinking or settling of phytoplankton is an important contribution to the overall mortality of the phytoplankton population, particularly in lakes and coastal oceanic waters. Published values of the sinking velocity of phytoplankton, mostly in quiescent laboratory conditions, range from 0.1 to 18.0 m/day. However, in some instances for certain species, such as dinoflagellates or buoyancy-retulating blue-greens, the settling velocity may be zero or negative. Furthermore, actual settling rates in natural waters are a complex phenomenon, affected by vertical turbulence, density gradients and the physiological state of the different species of phytoplankton. An important factor determining the physiological state of algae is nutrient availability. Bienfang et al. (1982) measured sinking rate response of four marine diatoms to depletion of nitrate, phosphate and silicate. All four species showed significant increase in sinking rate under conditions of silica depletion; one species showed increased settling rate under nitrate limitation. An analysis of field experiments by Culver and Smith (1989) indicated that low concentrations of nitrate, as well as light availability, affected diatom settling rates. Although the effective settling rate of phytoplankton is greatly reduced in a relatively shallow, well-mixed river or estuary, due to vertical turbulence, it still can contribute to the overall mortality of the algal population. In addition, the settling phytoplankton can be a significant source of nutrients to the sediments and can play an important role in the generation of SOD. For these reasons, a temperature- dependent term representing phyto-plankton settling has been included in the algal mortality expression, and may be written as follows:

$$k_{sP} = \left[\frac{V_{sPb}}{H} + \frac{V_{sPn}}{H} \cdot \left(1 - G_N(N)\right) \right] \cdot \theta_{base}^{(T-20)} \qquad (1\text{-}14)$$

where k_{sP} is the net effective algal loss rate due to settling (day^{-1}), v_{sPb} is the base settling velocity of phytoplankton (m/day), v_{sPn} is the nutrient dependent settling rate, (m/day), $G_N(N)$ is defined by Equation 1-12, and H is the depth of the segment, (m).

Zooplankton grazing may, depending upon time of the year and zooplankton biomass levels, be an important loss rate for phytoplankton. The loss term used to represent zooplankton grazing is as follows:

$$k_{grz}(T) = k_{grz}(20^{o}C) \cdot \theta_{grz}^{(T-20)} \qquad (1\text{-}15)$$

where $k_{grz}(T)$ is the temperature corrected loss rate due to zooplankton grazing and $k_{grz}(20°C)$ is the predation rate at 20°C. The units of k_{grz} are day^{-1}.

The total loss rate for phytoplankton is the sum of the three loss rates described above:

$$D_P = k_{PR}(T) + k_{sP} + k_{grz}(T) \qquad (1\text{-}16)$$

This completes the specification of the growth and death rates for phytoplankton (for the standard algal growth model) in terms of the physical variables: light, temperature and available nutrients. Table 1-1 summarizes the equations and model coefficients used in the standard version of the eutrophicaton model.

TABLE 1-1. STANDARD PHYTOPLANKTON GROWTH EQUATIONS

Phytoplankton Net Growth Rate

$$S_p = \left(G_{P\,max} \cdot G_T(T) \cdot G_I(I) \cdot G_N(N) - k_{PR}(T) - k_{sP} - k_{grz}(T)\right) \cdot P_c$$

Temperature Correction

Arrenhius Version

$$G_{Pmax}(T) = G_{Pmax}\ \theta_P^{(T-20)}$$

Optimum Temperature Version

$$G_{Pmax}(T) = G_{Pmax} e^{-\beta_1 (T - T_{opt})^2} \qquad T \leq T_{opt}$$

$$G_{Pmax}(T) = G_{Pmax} e^{-\beta_2 (T_{opt} - T)^2} \qquad T > T_{opt}$$

Light Reduction

$$G_I(I) = \frac{e}{k_e H}\left[\exp\left(\frac{-I_o(t)}{I_s} e^{-k_e H}\right) - \exp\frac{-I_o(t)}{I_s}\right]$$

$$k_e = k_{e_{base}} + k_c \cdot a_{cchl} \cdot P_c$$

Nutrient Uptake

$$G_N(N) = \mathrm{Min}\left(\frac{DIN}{K_{mN} + DIN}, \frac{DIP}{K_{mP} + DIP}, \frac{Si}{K_{mSi} + Si}\right)$$

DIN = dissolved inorganic nitrogen = $NH_4 + NO_2 + NO_3$,
DIP = dissolved inorganic phosphorus (PO_4),
Si = available silica

Algal Respiration

$$k_{PR}(T) = k_{PR}(20^o C) \cdot \theta_{PR}{}^{(T-20)}$$

or

$$k_{PR}(T) = r_g G_P + r_b \theta_{PR}{}^{(T-20)}$$

Algal Settling

$$k_{sP} = \left[\frac{V_{sPb}}{H} + \frac{V_{sPn}}{H} \cdot \left(1 - G_N(N)\right)\right] \cdot \theta_{base}^{(T-20)}$$

TABLE 1-1. STANDARD PHYTOPLANKTON NET GROWTH EQUATIONS
(Continued)

Zooplankton Grazing

$$k_{grz}(T) = k_{grz}(20^{o}C) \cdot \theta_{grz}^{(T-20)}$$

Exogenous Variables

Description	Notation
Total Extinction Coefficient	k_e
Base Extinction Coefficient	k_{ebase}
Total Daily Surface Solar Radiation	I_o
Temperature	T
Segment Depth	H

Rate Constants

Description	Notation	Winter Diatoms	Summer Assemblage	Units
Maximum Specific Growth Rate at T_{opt}	G_{Pmax}	1.7-2.5	2.0 - 3.0	day^{-1}
Temperature Coefficient	θ_P	1.068	1.068	
Temperature Optimum	T_{opt}	6-12	20 - 25	°C
Shaping parameters	β_1, β_2	0.003-0.006	0.003-0.006	
Phytoplankton Self-Light Attenuation	k_c	0.017	0.017	m^2/mg chl-a
Half-Saturation Constant for Nitrogen	K_{mN}	10.	10.	µgN/L
Half-Saturation Constant for Phosphorus	K_{mP}	1.	1.	µgP/L
Half-Saturation Constant for Silica	K_{mSi}	20.	2.	µgSi/L
Respiration Rate	$k_{PR}(20^oC)$	0.1-0.3	0.1-0.3	day^{-1}
Temperature Coefficient	θ_{PR}	1.047-1.068	1.047-1.068	
Cost of Photosynthesis	r_g	0.2 - 0.3	0.2 - 0.3	
Basal Respiration	r_b	0.01-0.03	0.01-0.03	/day
Base Algal Settling Rate	v_{sPb}	0.2-1.0	0.2-1.0	m/day
Nutrient Dependent Algal Settling Rate	v_{sPn}	0.5-1.0	0.5-1.0	m/day
Temperature Coefficient	θ_{base}	1.029	1.029	
Loss Due to Zooplankton Grazing	$k_{grz}(20^oC)$	0.05-0.10	0.05-0.10	/day
Temperature Coefficient	θ_{grz}	1.10	1.10	
Carbon/Chlorophyll Ratio	a_{cchl}	30-60.	75-100.	mgC/mg chl-a

1.2.2.2 Laws-Chalup Algal Growth Model

The second algal growth model available in this release of RCA draws directly from Laws and Chalup (1990) and an earlier modeling framework developed by Shuter (1979). The following paragraphs provide an overview of the Laws-Chalup model. In the Laws-Chalup model, the carbon in the phytoplankton cell is considered to be found in one of four compartments: structural carbon (S), reservoir or storage carbon (R), carbon associate with the light reactions (photochemical reactions) of photosynthesis (L), or carbon associated with the dark reactions (carbohydrate production and protein and lipid synthesis) of photosynthesis (D). Hence, total cell carbon, C = S + R + L + D. Chlorophyll is assumed to exist only in the L portion of the cell. Nutrients (nitrogen, phosphorus, and silica) are found in the S, L, and D portions of the cell and are assumed to be found in the same ratios in each of these pools. R is assumed to consist entirely of C storage products (carbohydrates and lipids) and hence contains no nutrients. The fraction of C allocated to structural purposes (S/C) is assumed to be constant and independent of growth conditions.

The steady-state gross photosynthetic rate per cell (ρ) is described by

$$\rho = G_{prl}\ L\ I = G_{prd}\ D \qquad (1\text{-}17)$$

where I is the incident irradiance; G_{prd} is the gross photosynthetic rate per unit D and is a constant; and G_{prl} is the gross rate of photosynthesis per unit L per unit light intensity and is a function of environmental conditions. Respiration losses are assumed to be described by

$$k_{PR} = k_{RB} + k_{RG}\ G_{prd}\ D \qquad (1\text{-}18)$$

where k_{RB} is the basal respiration rate per cell, i.e., the rate required to maintain the cell in the absence of growth, and k_{RG} is the growth-rate-dependent respiration coefficient (Laws and Bannister, 1980). The substrate for respiration is assumed to come from the R pool.

From the foregoing assumptions, it follows that the rate of nutrient assimilation f_N is constrained by

$$\frac{d}{dt}(S+L+D) = W_{Nx}\ f_N \qquad (1\text{-}19)$$

where W_{Nx} is the ratio of C to nutrient x (either nitrogen, phosphorus or silica). It also follows that

$$\frac{dC}{dt} = G_{prd}\ D - k_{RB} - k_{RG}\ G_{prd}\ D \qquad (1\text{-}20)$$

Under conditions of balanced growth it must be true that for any component X of the cell,

$$\mu = \frac{1}{X}\frac{dX}{dt} \qquad (1\text{-}21)$$

where μ is the growth rate in units of inverse time. Combining Equations (1-20) and (1-21) yields

$$\mu\,C = G_{prd}\,D - k_{RB} - k_{RG}\,G_{prd}\,D \tag{1-22}$$

Laws and Chalup also define the assumptions and conditions under which a nutrient saturated version of Equation 1-22 can be developed. The nutrient saturated growth rate, μ_{Pmax}, is of the form

$$\mu_{P\,max} = \frac{G_{prd}\left(1-k_{RG}\right)\left(1-S/C\right)I}{I + G_{prd}/G_{prls}} - \frac{k_{RB}}{C} \tag{1-23}$$

where G_{prls} is the nutrient-saturated value of G_{prl}. Laws and Chalup then account for the relationship between light and G_{prls} by use of Equation (1-24).

$$G_{prls} = \frac{G_{prlo}}{1 + I/I_s} \tag{1-24}$$

where G_{prlo} is the value of G_{prls} when $I = 0$, and Is is the value of I when $G_{prls} = 0.5G_{prlo}$.

As described in Section 1.2.2.1 Standard Algal Growth Model, in the natural environment, the light intensity or incident irradiance, I, to which the phytoplankton are exposed is not uniformly at the optimum value. The variations in light exposure that phytoplankton are exposed to due to position in the water column and daily variations to solar radiation that were detailed in Section 1.2.2.1 also apply in the Laws-Chalup growth model. Equations (1-10) and (1-11) are used to determine the diurnal variation in solar radiation at the surface of the water column, given the total solar radiation, and its attenuation through the water column, respectively.

One additional parameterization that is incorporated in the Laws-Chalup formulation is photo-adaptation by phytoplankton. Phytoplankton have been shown to be able to adapt to variations in light intensity (Steemann Nielsen et al., 1962; Steemann Nielsen and Park, 1964; Morel et al. 1987). Experimental data have indicated that phytoplankton may take several hours to two to four days to adapt to changes in light intensity. Therefore, the value of I_s, in Equation 1-24 is permitted to change as a function of the antecedent light history, according to the formula:

$$I_s = \left(I_{tot_{n-3}} + I_{tot_{n-2}} + I_{tot_{n-1}}\right)/3 \tag{1-25}$$

where:

$I_{tot_{n-3}}$ = total solar radiation three days preceding current model day,
$I_{tot_{n-2}}$ = total solar radiation two days preceding current model day,
$I_{tot_{n-1}}$ = total solar radiation one day preceding current model day.

Note: the use of the photo-adaptation formula is optional. If the user wishes to include photo-adaptation then he or she should set the appropriate I_{sat} in the "Constants" section of the model input to zero. Otherwise, if a non-zero value for I_{sat} is specified then photo-adaptation is ignored the user specified value for I_{sat} is applied in equations (1-9) or (1-24).

The nutrient saturated growth rate is then temperature-corrected using spatially dependent, time-dependent values of ambient water column temperature as computed by the hydrodynamic model. The temperature-corrected growth rate is computed usng either equation 1-8a or equations 1-8b and 1-8c. A principal difference between the winter diatom group and the summer assemblage is that the winter group has a much lower T_{opt} than does the summer assemblage. The nutrient saturated, temperature-corrected growth rate is then adjusted to reflect effects due to nutrient levels, as described earlier (Equation 1-12). Table 1-2 presents the equations used for algal growth for the Law-Chalup version of algal growth.

TABLE 1-2. LAWS-CHALUP PHYTOPLANKTON GROWTH EQUATIONS

Phytoplankton Net Growth Rate

$$S_p = (\mu_{Pmax}(T,I) \cdot G_N(N) - k_{RB} - k_{sP}(T) - k_{grz}(T)) \cdot P_c$$

Specific Growth Rate

$$G_p = \mu_{Pmax}(T,I) \cdot G_N(N)$$

Nutrient Saturated Growth Rate

$$\mu_{Pmax}(T_{opt}, I) = \frac{G_{prd} \cdot (1 - k_{RG}) \cdot (1 - S/C) \cdot I(z,t)}{G_{prd}/G_{prlo} + I(z,t)\ (1 + G_{prd}/I_s G_{prlo})} - k_{RB}$$

Temperature Correction

$$\mu_{Pmax}(T) = \mu_{Pmax}(T_{opt}) \cdot e^{-\beta_1 \cdot (T - T_{opt})^2} \qquad T \le T_{opt}$$

$$\mu_{Pmax}(T) = \mu_{Pmax}(T_{opt}) \cdot e^{-\beta_2 \cdot (T - T_{opt})^2} \qquad T > T_{opt}$$

Light Attenuation

$$I(z,t) = I_{surf}(t)\, e^{-k_e z}$$

Average Light

$$I_{ave} = \frac{I_{surf}(t)}{k_e H}\left(1 - e^{-k_e H}\right)$$

$$k_e = k_{e_{base}} + k_c \cdot a_{ChlC} \cdot P_c$$

$$I_{surf}(t) = \frac{I_{tot}}{0.635 \cdot f} \sin\left(\frac{\pi\left(t_d - t_{sunrise}\right)}{f}\right)$$

$$I_s = \left(I_{tot_{n-3}} + I_{tot_{n-2}} + I_{tot_{n-1}}\right)/3$$

TABLE 1-2. LAWS-CHALUP PHYTOPLANKTON GROWTH EQUATIONS (CONTINUED)

Chlorophyll to Carbon Ratio (a_{ChlC})

$$a_{ChlC} = \frac{1-(1-QF)\,(1-\mu/\mu_{Pmax})-S/C-(\mu+k_{RB}/C)/\left[(1-k_{RG})G_{prd}\right]}{W_{CChl}}$$

Nutrient Uptake

$$G_N(N) = \mathrm{Min}\left(\frac{DIN}{K_{mN}+DIN},\frac{DIP}{K_{mP}+DIP},\frac{Si}{K_{mSi}+Si}\right)$$

DIN = dissolved inorganic nitrogen = $NH_3 + NO_2 + NO_3$
DIP = dissolved inorganic phosphorus
Si = available silica

Endogenous Respiration

$$k_{PR} = \frac{k_{RB}+k_{RG}\cdot\mu}{1-k_{RG}}$$

$$\mu = G_N(N)\cdot\mu_{Pmax}$$

Algal Settling

$$k_{sP}(T) = \left(\frac{v_{sPb}}{H}+\frac{v_{sPn}}{H}\cdot(1-G_N(N))\right)\cdot\theta_{sP}^{(T-20)}$$

Zooplankton Grazing

$$k_{grz}(T) = k_{grz}(20^{o}C)\cdot\theta_{grz}^{(T-20)}$$

TABLE 1-2. LAWS-CHALUP PHYTOPLANKTON GROWTH EQUATIONS (CONTINUED)

Exogenous Variables

Description	Notation	Units
Total Extinction Coefficient	k_e	m^{-1}
Base Extinction Coefficient	k_{ebase}	m^{-1}
Total Daily Surface Solar Radiation	I_{tot}	langleys/day
Temperature	T	°C
Segment Depth	H	m
Fraction of Daylight	f	day
Time of Day	t_d	day
Time of Sunrise	$t_{sunrise}$	day

Rate Constants

Description	Notation	Winter Diatoms	Summer Assemblage	Units
Gross photosynthetic rate per unit D	G_{prd}	2.5	3.0	day^{-1}
Gross photosynthetic rate per unit L per unit light intensity in the limit of zero irradiance	G_{prlo}	0.28	0.28	m^2/mol quanta
Quotient of nutrient to carbon ratios at relative growth rates of 0 and 1	QF	0.85	0.85	
Effect of Temperature below T_{opt} on growth	β_1	0.004	0.004	
Effect of Temperature above T_{opt}	β_2	0.006	0.006	
Temperature Optimum	T_{opt}	8.	18.	°C
Phytoplankton Self-Shading Attenuation	k_c	0.017	0.017	m^2/mg chl-a
Half-Saturation Constant for Nitrogen	K_{mN}	0.010	0.010	mg N/L
Half-Saturation Constant for Phosphorus	K_{mP}	0.001	0.001	mg P/L
Half-Saturation Constant for Silica	K_{mSi}	0.020	0.005	mg Si/L
Growth Related Respiration Coefficient	k_{RG}	0.28	0.28	
Basal Respiration Rate	k_{RB}	0.03	0.036	day^{-1}
Base Algal Settling Rate	v_{sPb}	0.5	0.3	m/day
Nutrient Dependent Algal Settling Rate	v_{sPn}	1.0	0.7	m/day
Temperature Coefficient	θ_{sP}	1.027	1.027	
Loss Due to Zooplankton Grazing	k_{grz} (20°C)	0.1	0.1	day^{-1}
Temperature Coefficient	θ_{grz}	1.10	1.10	
Nutrient Saturated Carbon/Chlorophyll Ratio in L	W_{CChl}	40.	65.	mg C/mg chl-a
Ratio of Structural to Total Carbon	S/C	0.1	0.1	

1.2.3 Stoichiometry and Uptake Kinetics

A principal component in the mass balance equations for the nutrient systems included in the eutrophication framework is the nutrient uptake kinetics associated with algal growth (as defined via equations (1-5) through (1-25)). In order to quantify the nutrient uptake it is necessary to specify the population stoichiometry in units of nutrient uptake per mass of population synthesized. For carbon as the unit of population biomass, the relevant ratios are the mass of nitrogen, phosphorus and silica per unit mass of carbon.

This version of the integrated eutrophication model includes two variable algal stoichiometry formulations as well as the more traditional constant stoichiometry formulation. The variable stoichiometry formulation allows internal algal nutrient levels to vary as a function of the external nutrient levels. This process is sometimes referred to as "luxury nutrient uptake". That is, when external nutrient levels are in surplus the internal nutrient to carbon ratio increases thereby allowing internal storage of nutrients. The reverse occurs when external nutrient levels are low and are approaching the nutrient half saturation constant. In this case, the internal nutrient to carbon ratios decrease and the algal cell can continue to grow at low external nutrient levels.

1.2.3.1 Algal Stoichiometry and Uptake Kinetics - Standard Algal Growth Model

As mentioned above, two forms of variable nutrient stoichiometry are included in the integrated eutrophication model. The first is based on an emphirical formulation developed for the Chesapeake Bay model (Cerco, 1995). This formulation is presented graphically in Figure 1-3 for the carbon to phosphorus ratio from measurements collected in upper Chesapeake Bay.

A generalized variable stoichiometry formulation, based on the Chesapeake Bay model, may be written for a dissolved nutrient (DIX) as follows:

$$\frac{C}{X} = X_1 + (X_2 - X_1)e^{-X_3 \cdot DIX} \tag{1-26}$$

where:

$\frac{C}{X}$ = carbon to nutrient ratio,

X_1 = nutrient saturated, carbon to nutrient ratio,

X_2 = nutrient limited, carbon to nutrient ratio (maximum),

X_3 = coefficient that determines the rate at which the carbon to nutrient ratio changes as a function of the ambient nutrient concentration, DIX,

DIX = dissolved concentration of available nutrient (either DIN, DIP, or DSi).

Table 1-3 lists the range in nitrogen, phosphorus and silica variable-stiochiometry coefficients used in previous modeling studies conducted by HydroQual.

TABLE 1-3. VARIABLE STOICHIOMETRY COEFFICIENTS - STANDARD ALGAL GROWTH MODEL

	Winter Assemblage	Summer Assemblage
Nitrogen		
CRBN1 (mgC/mgN)	5.2-5.67	4-5.67
CRBN2 (mgC/mgN)	6.5-7.20	7.5-10.0
CRBN3 (L/mgN)	10-15	10-15
Phosphorus		
CRBP1 (mgC/mgP)	25-40	25-40
CRBP2 (mgC/mgP)	90	90
CRBP3 (L/mgP)	100-200	40-200
Silica		
CRBS1 (mgC/mgSi)	2.2-3.0	5.-10.
CRBS2 (mgC/mgSi)	8-15	10-25
CRBS3 (L/mgSi)	12-30	5-10

1.2.3.2 Algal Stoichiometry and Uptake Kinetics - Laws-Chalup Algal Growth Model

Lacking extensive measurements of the particulate forms of carbon, nitrogen, phosphorus and biogenic silica, many modeling studies have assumed that phytoplankton are comprised of carbon and nutrients which approximate Redfield ratios; i.e., 106C:16N:1P (atomic), under nutrient saturated conditions. However, while the use of Redfield ratios may be appropriate under nutrient saturated conditions, it has been shown (Anita et al., 1963; Caperon and Meyer, 1972; Chalup and Laws, 1990) that algae change their cellular composition or stoichiometry as a function of nutrient status. This is accounted for in the Laws/Chalup model via the following equations:

$$\begin{aligned} N_x : C &= \left[QF + (1 - QF)\ (\mu / \mu_{P\max} \right] / W_{Cx} \\ &= 1 / W_{Cx} \text{ when } \mu = \mu_{P\max} \end{aligned} \tag{1-27}$$

and

$$\mathrm{Chl:C} = \frac{1-(1-\mathrm{QF})\,(1-\mu/\mu_{\mathrm{Pmax}}) - \mathrm{S/C} - (\mu + \mathrm{k_{RB}}/\mathrm{C})/\left[(1-\mathrm{k_{RG}})\,\mathrm{G_{prd}}\right]}{\mathrm{W_{chl}}} \tag{1-28}$$

$$= \left\{1-\mathrm{S/C} - (\mu_{\mathrm{Pmax}} + \mathrm{k_{RB}C})/\left[(1-\mathrm{k_{RG}})\,\mathrm{G_{prd}}\right]\right\}/\mathrm{W_{chl}} \text{ when } \mu = \mu_{\mathrm{Pmax}}$$

where:

N_x:C = the ratio of nutrient x (nitrogen, phosphorus or silica) to carbon,
QF = quotient of N_x:C values at relative growth rates of 0 and 1,
μ = the nutrient corrected growth rate ($\mu = \mu_{Pmax}$ GN(N)),
W_{Cx} = the ratio of C to nutrient x in S, L, D,
Chl:C = the ratio of chlorophyll-a to C in P,
W_{Chl} = the ratio of C to chlorophyll-a in P.

The latter equation accounts for changes in the chlorophyll to carbon ratio both as a function of nutrient status and light. Equations 1-27 and 1-28 provide the equilibrium carbon to nutrient and carbon to chlorophyll ratios. However, as has been shown from experimental studies, there is a time period over which it takes the phytoplankton to reach new equilibrium conditions in response to changes in nutrient status and/or available light. This is accounted for by use of the following equations:

$$\frac{dN_x:C^n}{dt} = k_{eq}\left(N_x:C^n_{eq} - N_x:C^n\right) \tag{1-29}$$

$$N_x:C^{n+1} = N_x:C^n + dt\,\frac{dN_x:C^n}{dt} \tag{1-30}$$

and

$$\frac{d\mathrm{Chl}:C^n}{dt} = k_{eq}\left(\mathrm{Chl}:C^n_{eq} - \mathrm{Chl}:C^n\right) \tag{1-31}$$

$$\mathrm{Chl}:C^{n+1} = \mathrm{Chl}:C^n + dt\,\frac{d\mathrm{Chl}:C^n}{dt} \tag{1-32}$$

where:

$N_x:C^n$, $N_x:C^{n+1}$ = the nutrient to carbon ratios at time step n and n+1, respectively,
$N_x:C^n_{eq}$ = the equilibrium nutrient to carbon ratio at time step n, as determined from Equation 1-27,
k_{eq} = a constant which determines the time to achieve equilibrium,
$\mathrm{Chl}:C^n$, $\mathrm{Chl}:C^{n+1}$ = the chlorophyll to carbon ratios at time step n and n+1, respectively,
$\mathrm{Chl}:C^n_{eq}$ = the equilibrium chlorophyll to carbon ratio at time step n, as determined from Equation 1-28,
dt = length of time step.

The Laws-Chalup algal growth model evaluates the nutrient to carbon and chlorophyll to carbon ratios to be used form the next time level based on the ratios at the current time level and the equilibrium ratios, determined from Equations 1-27 and 1-28, based upon environmental conditions at the current time level. A value of 1/day was chosen for k_{eq}, based on the literature (Steeman Nielsen and Park, 1964; Anita et al., 1963; Caperon and Meyer, 1972). This corresponds to an equilibrium time of approximately 3 days. This value has been "hard-wired" in the computer code. Table 1-4 contains the stoichiometric coefficients used in the Massachusetts Bays application of RCA.

TABLE 1-4 VARIABLE STOICHIOMETRY COEFFICIENTS -
LAWS-CHALUP ALGAL GROWTH MODEL

	Winter Assemblage	Summer Assemblage
Nitrogen		
W_{CN}	5.67 (6.67(1) - 16.2(2))	5.67 (6.67(1) - 16.2(2))
Phosphorus		
W_{CP}	40.(47(1) - 114(2))	40.(47(1) - 114(2))
Silica		
W_{csi}	2.5(2.94(1) - 7.14(2))	7.0(8.2(1) - 20.(2))
QF	0.85(1)	0.85(1)
quotient of nutrient to carbon ratio at relative growth rates of 0 and 1		

(1) maximum C to nutrient ratio at nutrient-limiting conditions using Massachusetts Bays model coefficient of 0.85 for QF

(2) maximum C to nutrient ratio at nutrient-limiting conditions using Laws-Chalup (1990) model coefficient f 0.35 for QF

Figure 1-4 presents a comparison of the carbon to nitrogen ratios obtained using the standard eutrophication variable stoichiometry foundation (Eqn. 1-26) using coefficients used in HydroQual studies versus that proposed by Laws and Chalup (Eqn. 1-27). It is important to note, however, that the coefficient set used by Laws and Chalup was for a single algal species and that a coefficient set that did not produce as sharp a curve was used by HydroQual in its Massachusetts Bay study (1995, 2003).

1.2.3.3 Nutrient Cycling

Once the stoichiometric ratios have been determined, the mass balance equations may be written for the nutrients in much the same way as for the phytoplankton biomass. The principal processes determining the distribution of nutrients among the various pools are: the uptake of inorganic nutrients by phytoplankton for cell growth, the release of organic nutrients by algal respiration and predation processes, and the recycling of organic nutrients to inorganic forms via bacterial hydrolysis and mineralization.

In their work on Lake Huron and Saginaw Bay, Di Toro and Matystick (1980) proposed a nutrient recycle formulation that was a function of the localized phytoplankton population. Drawing from an analysis of available field data and citing the work of others (Hendry, 1977; Lowe, 1976; Henrici, 1938; Menon et al., 1972; and Rao, 1976) that indicated bacterial biomass increased as phytoplankton biomass increased, the mechanism chosen, saturating recycle, was a compromise. This compromise was between the conventional first-order temperature corrected mechanism and a second-order recycle mechanism, in which the recycle rate is directly proportional to the phytoplankton biomass present, as indicated in pure culture, bacteria seeded laboratory studies (Jewell and McCarty 1971). The various relationships may be written:

$$\text{First} - \text{order recycle}: \quad k(T) = k'(20^{o}C)\,\theta^{T-20} \tag{1-33a}$$

$$\text{Second} - \text{order recycle}: \quad k(T) = k''(20^{o}C)\,\theta^{T-20} \cdot P_c \tag{1-33b}$$

$$\text{Saturating recycle}: \quad k(T) = k'(20^{o}C)\,\theta^{T-20} \cdot \frac{P_c}{K_{mP_c} + P_c} \tag{1-33c}$$

Saturating recycle permits second-order dependency at low phytoplankton concentrations, when $P_c << K_{mPc}$, where K_{mPc} is the half saturation constant for recycle. It also permits first-order recycle when the phytoplankton concentrations greatly exceed the half saturation constant. Basically, this mechanism employs a second order recycle that slows the recycle rate if the algal population is small, but does not permit the rate to increase continuously as phytoplankton concentrations increase. The assumption is that at higher population levels, other factors are limiting the recycle kinetics so that it proceeds at its maximum first-order rate.

1.2.3.4 Organic Carbon

Seven organic carbon state variables are considered: reactive particulate organic (RePOC), reactive dissolved organic (ReDOC), labile dissolved (LDOC), refractory dissolved (RDOC), labile particulate (LPOC), refractory particulate (RPOC) and dissolved algal exudate (ExDOC). Reactive, labile and refractory distinctions are based upon the time scale of oxidation or decomposition. Reactive organic carbon decomposes on a time scale of days to a week or two and is meant to be used for CSO carbon and a portion of the organic carbon discharged from wastewater treatment plants; labile organic carbon decomposes on the time scale of several weeks to a month or two; refractory organic carbon decomposes on the order of months to a year. Reactive and labile organic carbon decompose primarily in the water column or else rapidly in the sediments. Refractory organic carbon decomposes much more slowly, almost entirely in the sediments.

Reactive particulate organic carbon (RePOC) is assumed to have a very high settling rate that is a function of RePOC itself (representing floculation). The underlying assumption is that at elevated concentrations flocculations occurs, thereby enhancing the settling rate of this form of organic carbon. Equation 1-34 is used to determine the settling rates as a function of REPOC (Figure 1-5 illustrates REPOC settling rate as a function of REPOC and the two model coefficients β and C_{ref}). Information from settling column tests can be used to guide the selection of appropriate model coefficients, but it is important to (1) remember that settling column tests are usually conducted under quiescent conditions that may not occur in natural systems and (2) the choice of a maximum settling rate should be made remembering that the maximum rate may influence the integration step-size. For example, assuming a maximum rate of 50 m/day

$$v = \min\left[v_{max}, v_{min} + (v_{max} - v_{min})\left(\frac{RePOC}{C_{ref}}\right)^{\beta} \right] \tag{1-34}$$

a water column depth of 1 m and a ten layer sigma-level grid would require a time step of about 2.9 minutes or less to ensure numerical stability.

where

v = settling rate, (m/day)
v_{max} = maximum settling rate, (m/day)
v_{min} = maximum settling rate, (m/day)
RePOC = concentration of reactive (CSO) POC, (mg/L)
C_{ref} = reference concentration of RePOC, (mg/L)
β = power exponent for settling function

The principal sources of organic carbon are anthropogenic inputs and natural runoff, and detrital algal carbon, which is produced as a result of predation. Zooplankton take up and redistribute algal carbon to the organic carbon pools via grazing, assimilation, respiration and excretion. Since zooplankton are not directly included in the model, the redistribution of algal carbon by zooplankton is simulated by empirical distribution coefficients. An additional term, representing the excretion of DOC by phytoplankton during photosynthesis, is included in the model. This algal exudate is very reactive and has a time constant similar to the reactive DOC.

The decomposition of organic carbon is assumed to be temperature and bacterial biomass mediated. Since bacterial biomass is not directly included within the model framework, phytoplankton biomass is used as a surrogate variable. Table 1-5 presents the reaction rate terms and range of coefficients for each of the organic carbon pools considered in the model framework.

TABLE 1-5. ORGANIC CARBON REACTION EQUATIONS
(Numbering scheme refers to the variable list in Section 1.1.2)

Refractory Particulate Organic Carbon (RPOC)

$$S_{18} = f_{RPOC} \cdot k_{grz}(T) \cdot P_c - k_{18,20}\,\theta_{18,20}{}^{T-20} \cdot RPOC \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{v_{s18}}{H} \cdot RPOC$$

Labile Particulate Organic Carbon (LPOC)

$$S_{19} = f_{LPOC} \cdot k_{grz}(T) \cdot P_c - k_{19,21}\,\theta_{19,21}{}^{T-20} \cdot LPOC \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{v_{s19}}{H} \cdot LPOC$$

Refractory Dissolve Organic Carbon (RDOC)

$$S_{20} = f_{RDOC} \cdot k_{grz}(T) \cdot P_c - k_{18,20}\,\theta_{18,20}{}^{T-20} \cdot RPOC \cdot \frac{P_c}{K_{mP_c} + P_c}$$

$$- k_{20,0}\,\theta_{20,0}{}^{T-20} \cdot RDOC \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO} + DO}$$

Labile Dissolved Organic Carbon (LDOC)

$$S_{21} = f_{LDOC} \cdot k_{grz}(T) \cdot P_c - k_{19,21}\,\theta_{19,21}{}^{T-20} \cdot LPOC \cdot \frac{P_c}{K_{mP_c} + P_c}$$

$$- k_{21,0}\,\theta_{21,0}{}^{T-20} \cdot LDOC \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO} + DO} \cdot \frac{LDOC}{K_{mLDOC} + LDOC}$$

$$-\frac{5}{4} \cdot \frac{12}{14} \cdot k_{15,0}\,\theta_{15,0}{}^{T-20} \cdot NO_2 + NO_3 \cdot \frac{K_{NO_3}}{K_{NO_3} + DO}$$

TABLE 1-5. ORGANIC CARBON REACTION EQUATIONS
(Numbering scheme refers to the variable list in Section 1.1.2)
(Continued)

Algal Exudate Dissolved Organic Carbon (ExDOC)

$$S_{22} = f_{ExPP} \cdot G_P \cdot P_c - k_{22,0}\theta_{22,0}{}^{T-20} \cdot ExDOC \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO} + DO} \cdot \frac{ExDOC}{K_{mLDOC} + ExDOC}$$

Reactive Particulate Organic Carbon (RePOC)

$$S_{23} = -k_{23,24}\theta_{23,24}{}^{T-20} \cdot \mathrm{Re\,POC} \cdot \frac{P_c}{k_{mp_c} + P_c} - \min\left[v_{24\max},\ v_{24\min} + \left(v_{24\max} - v_{24\min}\right)\left(\frac{\mathrm{Re\,POC}}{C_{ref}}\right)^{\beta}\right] \cdot \mathrm{Re\,POC}$$

Reactive Dissolved Organic Carbon (ReDOC)

$$S_{24} = -k_{23,24}\theta_{23,24}{}^{T-20} \cdot \mathrm{Re\,POC} \cdot \frac{P_c}{k_{mp_c} + P_c} \cdot k_{24,0}\theta_{24,0}{}^{T-20} \cdot \mathrm{Re\,DOC} \cdot \frac{P_c}{k_{mp_c} + P_c} \cdot \frac{DO}{K_{DO} + DO} \cdot \frac{\mathrm{Re\,DOC}}{K_{mLDOC} + \mathrm{Re\,DOC}}$$

TABLE 1-5. ORGANIC CARBON REACTION EQUATIONS
(Numbering scheme refers to the variable list in Section 1.1.2)

Description	Notation	Value	Units
Phytoplankton Biomass	P_c	-	mgC/L
Specific Phytoplankton Growth Rate	G_P	Eq. 1-5	day^{-1}
Segment depth	H	-	m
Dissolved Oxygen	DO	-	mgO_2/L
Half Saturation Constant for Phytoplankton Limitation	K_{mPc}	0.05	mgC/L
Fraction of Grazed Organic Carbon Recycle to:			
the LPOC pool	f_{LPOC}	0.30-0.40	
the RPOC pool	f_{RPOC}	0.10-0.15	
the LDOC pool	f_{LDOC}	0.35-0.45	
the RDOC pool	f_{RDOC}	0.10-0.15	
Note: the sum of $f_{LPOC} + f_{RPOC} + f_{LDOC} + f_{RDOC}$ must equal 1.0			
Fraction of Primary Productivity Going to the Algal Exudate DOC pool	f_{ExPP}	0.10-0.15	
Hydrolysis Rate for RPOC	$k_{18,20}$	0.007-0.01	day^{-1}
Temperature Coefficient	$\theta_{18,20}$	1.08	
Settling Rate of RPOC	v_{s18}	0.5-1.0	m/day
Hydrolysis Rate for LPOC	$k_{19,21}$	0.07-0.10	day^{-1}
Temperature Coefficient	$\theta_{19,21}$	1.08	
Settling Rate of LPOC	v_{s19}	0.5-1.0	m/day
Oxidation Rate of RDOC	$k_{20,0}$	0.007-0.01	day^{-1}
Temperature Coefficient	$\theta_{20,0}$	1.08	
Oxidation Rate LDOC	$k_{21,0}$	0.10-0.15	day^{-1}
Temperature Coefficient	$\theta_{21,0}$	1.08	
Oxidation Rate of ReDOC	$k_{22,0}$	0.25-0.35	day^{-1}
Temperature Coefficient	$\theta_{22,0}$	1.047	
Oxidation Rate of ExDOC	$k_{23,0}$	0.1	day^{-1}
Temperature Coefficient	$\theta_{23,0}$	1.08	
Half Saturation for Oxygen Limitation	k_{DO}	0.2	mgO_2/L
Michaelis Constant for LDOC	K_{mLDOC}	0.1	mgC/L
Minimum RePOC settling rate	$v_{24\,min}$	0.5	m/day
Enhanced RePOC settling rate (due to floculation)	v_{24max}	25	m/day
Reference (or normalizing term)	C_{Ref}	10	mgC/day
Power function	β	1.2	

1.2.3.5 Phosphorus

The eutrophication model includes five principal phosphorus forms: labile and refractory dissolved organic (LDOP and RDOP, respectively), labile and refractory particulate organic (LPOP and RPOP, respectively), and DIP. Inorganic phosphorus is utilized by phytoplankton for growth and phosphorus is returned to the various organic and inorganic forms via respiration and predation. A fraction of the phosphorus released during phytoplankton respiration and predation is in the inorganic form and readily available for uptake by other viable algal cells. The remaining fraction released is in the dissolved and particulate organic forms. The organic phosphorus must undergo a mineralization or bacterial decomposition into inorganic phosphorus before it can be used by phytoplankton. Table 1-6 presents the reaction rate terms for each of the five phosphorus forms.

1.2.3.6 Nitrogen

The kinetic structure for nitrogen is similar to that for the phosphorus system. Table 1-7 summarizes the terms used in the nitrogen system kinetics. During algal respiration and death, a fraction of the cellular nitrogen is returned to the inorganic pool in the form of NH_3. The remaining fraction is recycled to the dissolved and particulate organic nitrogen pools. Organic nitrogen undergoes a bacterial decomposition, the end-product of which is NH_4. Ammonia nitrogen, in the presence of nitrifying bacteria and oxygen, is converted to nitrite nitrogen and subsequently nitrate nitrogen (nitrification). Both ammonia and nitrate are available for uptake and are used in cell growth by phytoplankton; however, for physiological reasons, the preferred form is NH_4. The ammonia preference term takes the following form:

$$\begin{aligned}\alpha_{NH_4} &= NH_4 \cdot \frac{NO_2 + NO_3}{(K_{mN} + NH_4)\cdot(K_{mN} + NO_2 + NO_3)} \\ &+ NH_4 \cdot \frac{K_{mN}}{(NH_4 + NO_2 + NO_3)\cdot(K_{mN} + NO_2 + NO_3)}\end{aligned} \tag{1-35}$$

The behavior of this equation for a Michaelis value, K_{mN}, of 10 μgN/L, is illustrated on Figure 1-6. The behavior of Equation 1-35 is most sensitive at low values of ammonia or nitrate. For a given concentration of ammonia, as the available nitrate increases above approximately the Michaelis limitation, the preference for ammonia reaches a plateau. Also, as the concentration of available ammonia increases, the plateau occurs at values closer to unity, that is, total preference for ammonia. The process of nitrification in natural waters is carried out by aerobic autotrophs, *Nitrosomonas* and *Nitrobacter*, in particular. It is a two-step process with *Nitrosomonas* bacteria responsible for the conversion of ammonia to nitrite (NO_2) and *Nitrobacter* responsible for the subsequent conversion of nitrite to nitrate (NO_3). Essential to this reaction process are aerobic conditions. In order to reduce the number of state variables required in the modeling framework, it was decided to incorporate nitrite and nitrate together as a single state variable. Therefore, the process of nitrification is assumed to be approximated by a first-order reaction rate that is a function of the water column dissolved oxygen concentration and ambient temperature.

TABLE 1-6. PHOSPHORUS REACTION RATES
(Numbering scheme refers to the variable list in Section 1.1.2)

Refractory Particulate Organic Phosphorus (RPOP)

$$\begin{aligned} S_5 &= a_{PC} \cdot f_{RPOP} \cdot \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_c - k_{5,7}\, \theta_{5,7}^{\;T-20} \cdot RPOP \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &\quad - \frac{v_{s5}}{H} \cdot RPOP \end{aligned}$$

Labile Particulate Organic Phosphorus (LPOP)

$$\begin{aligned} S_6 &= a_{PC} \cdot f_{LPOP} \cdot \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_c - k_{6,8}\, \theta_{6,8}^{\;T-20} \cdot LPOP \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &\quad - \frac{v_{s6}}{H} \cdot LPOP \end{aligned}$$

Refractory Dissolved Organic Phosphorus (RDOP)

$$\begin{aligned} S_7 &= a_{PC} \cdot f_{RDOP} \cdot \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_c + k_{5,7}\, \theta_{5,7}^{\;T-20} \cdot RPOP \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &\quad - k_{7,9} \theta_{7,9}^{\;T-20} \cdot RDOP \cdot \frac{P_c}{K_{mP_c} + P_c} \end{aligned}$$

Labile Dissolved Organic Phosphorus (LDOP)

$$\begin{aligned} S_8 &= a_{PC} \cdot f_{LDOP} \cdot \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_c + k_{6,8}\, \theta_{6,8}^{\;T-20} \cdot LPOP \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &\quad - k_{8,9}\, \theta_{8,9}^{\;T-20} \cdot LPOP \cdot \frac{P_c}{K_{mP_c} + P_c} \end{aligned}$$

TABLE 1-6. PHOSPHORUS REACTION RATES
(Continued)

Dissolved Inorganic Phosphorus (DIP)

$$\begin{aligned} S_9 &= a_{PC} \cdot f_{DIP} \cdot \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_c \\ &\quad + \left(k_{7,9}\,\theta_{7,9}^{\,T-20} \cdot RDOP + k_{8,9}\,\theta_{8,9}^{\,T-20} \cdot LDOP\right) \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &\quad - a_{PC} \cdot \left(1 - f_{ExPP}\right) \cdot G_P \cdot P_c \end{aligned}$$

TABLE 1-6. PHOSPHORUS REACTION RATES
(Continued)

Description	Notation	Value	Units
Phytoplankton Biomass	P_c	-	mgC/L
Temperature Corrected Algal Respiration Rate	$k_{PR}(T)$	Eq. 1-11a	day^{-1}
Temperature Corrected Grazing Rate	$k_{grz}(T)$	Eq. 1-13	day^{-1}
Specific Phytoplankton Growth Rate	G_P	Eq. 1-5	day^{-1}
Phosphorus to Carbon Ratio	a_{PC}	Table 1-2	mgP/mgC
Fraction of Primary Productivity Going to the Algal Exudate DOC pool	f_{ExPP}	0.1	
Fraction of Respired and Grazed Algal Phosphorus Recycled to			
the LPOP pool	f_{LPOP}	0.25-0.35	
the RPOP pool	f_{RPOP}	0.10-0.15	
the LDOP pool	f_{LDOP}	0.10-0.15	
the RDOP pool	f_{RDOP}	0.100.15	
the DIP pool	f_{DIP}	0.20-0.45	
Note: the sum of $f_{LPOP} + f_{RPOP} + f_{LDOP} + f_{RDOP} + f_{DIP}$ must equal 1.0			
RPOP Hydrolysis Rate at 20°C	$k_{5,7}$	0.007-0.01	day^{-1}
Temperature Coefficient	$\theta_{5,7}$	1.08	
RPOP Settling Rate	v_{s5}	0.5-1.0	m/day
LPOP Hydrolysis Rate at 20°C	$k_{6,8}$	0.085-0.10	day^{-1}
Temperature Coefficient	$\theta_{6,8}$	1.08	
LPOP Settling Rate	v_{s6}	0.5-1.0	m/day
RDOP Mineralization Rate at 20°C	$k_{7,9}$	0.01-0.02	day^{-1}
Temperature Coefficient	$\theta_{7,9}$	1.08	
LDOP Mineralization Rate at 20°C	$k_{8,9}$	0.1-0.2	day^{-1}
Temperature Coefficient	$\theta_{8,9}$	1.08	

TABLE 1-7. NITROGEN REACTION RATES
(Numbering scheme refers to the variable list in Section 1.1.2)

Refractory Particulate Organic Nitrogen (RPON)

$$S_{10} = a_{NC} \cdot f_{RPON} \cdot \left(k_{PR}(T) + k_{grz}\ (T)\right) \cdot P_c - k_{10,12}\,\theta_{10,12}{}^{T-20} \cdot RPON \cdot \frac{P_c}{K_{mP_c} + P_c}$$
$$- \frac{V_{s10}}{H} \cdot RPON$$

Labile Particulate Organic Nitrogen (LPON)

$$S_{11} = a_{NC} \cdot f_{LPON} \cdot \left(k_{PR}(T) + k_{grz}\ (T)\right) \cdot P_c - k_{11,13}\,\theta_{11,13}{}^{T-20} \cdot LPON \cdot \frac{P_c}{K_{mP_c} + P_c}$$
$$- \frac{V_{s11}}{H} \cdot LPON$$

Refractory Dissolved Organic Nitrogen (RDON)

$$S_{12} = a_{NC} \cdot f_{RDON} \cdot \left(k_{PR}(T) + k_{grz}\ (T)\right) \cdot P_c + k_{10,12}\,\theta_{10,12}{}^{T-20} \cdot RPON \cdot \frac{P_c}{K_{mP_c} + P_c}$$
$$- k_{12,14}\,\theta_{12,14}{}^{T-20} \cdot RDON \cdot \frac{P_c}{K_{mP_c} + P_c}$$

Labile Dissolved Organic Nitrogen (LDON)

$$S_{13} = a_{NC} \cdot f_{LDON} \cdot \left(k_{PR}(T) + k_{grz}\ (T)\right) \cdot P_c + k_{11,13}\,\theta_{11,13}{}^{T-20} \cdot LPON \cdot \frac{P_c}{K_{mP_c} + P_c}$$
$$k_{13,14}\,\theta_{13,14}{}^{T-20} \cdot LDON \cdot \frac{P_c}{K_{mP_c} + P_c}$$

TABLE 1-7. NITROGEN REACTION RATES
(Continued)

Ammonia Nitrogen (NH_4)

$$\begin{aligned} S_{14} = {} & a_{NC} \cdot f_{NH_4} \cdot \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_c \\ & + \left(k_{12,14}\,\theta_{12,14}{}^{T-20} \cdot RDON + k_{13,14}\,\theta_{13,14}{}^{T-20} \cdot LDON\right) \cdot \frac{P_c}{K_{mP_c} + P_c} \\ & - a_{NC} \cdot \alpha_{NH_4} \cdot (1 - f_{ExPP}) \cdot G_P \cdot P_c - k_{14,15}\,\theta_{14,15}{}^{T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO} \end{aligned}$$

Nitrite + Nitrate Nitrogen (NO_2+ NO_3)

$$\begin{aligned} S_{15} = {} & k_{14,15}\,\theta_{14,15}{}^{T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO} - a_{NC} \cdot \left(1 - \alpha_{NH_4}\right) \cdot \\ & (1 - f_{ExPP}) \cdot G_P \cdot P_c - k_{15,0}\,\theta_{15,0}{}^{T-20} \cdot NO_2 + NO_3 \cdot \frac{K_{NO_3}}{K_{NO_3} + DO} \end{aligned}$$

TABLE 1-7. NITROGEN REACTION RATES
(Continued)

Description	Notation	Value	Units
Phytoplankton Biomass	P_c	-	mgC/L
Temperature Corrected Algal Respiration Rate	$k_{PR}(T)$	cf Eq. 1-11a	day^{-1}
Temperature Corrected Grazing Rate	$k_{grz}(T)$	cf Eq. 1-13	day^{-1}
Specific Phytoplankton Growth Rate	G_P	cf Eq. 1-5	day^{-1}
Nitrogen to Carbon Ration	a_{NC}	cf Table 1-2	mgN/mgC
Fraction of Primary Productivity Going to the Algal Exudate DOC pool	f_{ExPP}	0.1	
Fraction of Respired and Grazed Algal Nitrogen Recycled to			
The LPON pool	f_{LPON}	0.30-0.35	
the RPON pool	f_{RPON}	0.10-0.15	
the LDON pool	f_{LDON}	0.125-0.15	
the RDON pool	f_{RDON}	0.125-0.20	
the NH_4 pool	f_{NH4}	0.15-0.35	
Note: the sum of $f_{LPON} + f_{RPON} + f_{LDON} + f_{RDON} + f_{NH4}$ must equal 1.0			
RPON Hydrolysis Rate at 20°C	$k_{10,12}$	0.007-0.01	day^{-1}
Temperature Coefficient	$\theta_{10,12}$	1.08	
RPON Settling Rate	v_{s10}	0.5-1.0	m/day
LPON Hydrolysis Rate at 20°C	$k_{11,13}$	0.05-0.07	day^{-1}
Temperature Coefficient	$\theta_{11,13}$	1.08	
LPON Settling Rate	v_{s11}	0.5-1.0	m/day
RDON Mineralization Rate at 20°C	$k_{12,14}$	0.0080.01	day^{-1}
Temperature Coefficient	$\theta_{12,14}$	1.08	
LDON Mineralization Rate at 20°C	$k_{13,14}$	0.085-0.10	day^{-1}
Temperature Coefficient	$\theta_{13,14}$	1.08	
Nitrification Rate at 20°C	$k_{14,15}$	0.05-0.10	day^{-1}
Temperature Coefficient	$\theta_{14,15}$	1.08	
Half Saturation Constant for Oxygen Limitation	K_{nitr}	1.0	$mg0_2/L$
Denitrification Rate at 20°C	$K_{15,0}$	0.05-0.4	day^{-1}
Temperature Coefficient	$\theta_{15,0}$	1.045	
Michaelis Constant for Denitrification	K_{NO_3}	0.1	$mg0_{2/L}$

Denitrification refers to the reduction of NO_3 to N_2 and other gaseous products such as N_2O and NO. This process is carried out by a large number of heterotrophic, facultative anaerobes. Under normal aerobic conditions found in the water column, these organisms utilize oxygen to oxidize organic material. However, under the anaerobic conditions found in the sediment bed or during extremely low oxygen conditions in the water column, these organisms are able to use NO_3 as the electron acceptor. The process of denitrification is included in the modeling framework simply as a sink of nitrate. This can always occur in the anaerobic sediment layer. In the water column, however, denitrification should only occur under extremely low dissolved oxygen conditions. This is accomplished computationally by modifying the linear first-order denitrification rate by the expression $K_{NO3}/(K_{NO3} + DO)$. This expression is similar to the Michaelis-Menton expression; for concentrations of dissolved oxygen greater than 1 mg/L, the expression reduces denitrification to near zero, whereas for dissolved oxygen levels less than 0.1mg/L, this expression permits denitrification to occur. Table 1-7 presents the state-variable equations for the six nitrogen forms utilized in the model framework.

1.2.3.7 Silica

Two silica state-variables are considered: available (Si) and unavailable or particulate biogenic (SiU). Available silica is dissolved and is utilized by diatoms during growth for their cell structure. Unavailable or particulate biogenic silica is produced from diatom respiration and diatom grazing by zooplankton. Particulate biogenic silica undergoes mineralization to available silica or settles to the sediment from the water column. Table 1-8 presents the state-variable equations for the two silica forms utilized in the model framework.

1.2.3.8 Dissolved Oxygen

A by-product of photosynthetic carbon fixation is the production of dissolved oxygen. The rate of oxygen production and nutrient uptake is proportional to the growth rate of the phytoplankton, since its stoichiometry is fixed. An additional source of oxygen from algal growth occurs when the available ammonia nutrient source is exhausted and the phytoplankton begin to utilize the available nitrate. This additional oxygen source can be seen by comparing equations 1-36a and 1-36b (Morel, 1983).

$$\begin{aligned} &106\ CO_2 + 16\ NH_4^+ + H_2PO_4^- + 106\ H_2O \\ &\qquad \Rightarrow \text{Protoplasm} + 106\ \ O_2 + 15H^+ \end{aligned} \tag{1-36a}$$

$$\begin{aligned} &106\ CO_2 + 16\ NO_3^- + H_2PO_4^- + 122\ H_2O + 17H + \\ &\qquad \Rightarrow \text{Protoplasm} + 138\ \ O_2 \end{aligned} \tag{1-36b}$$

The above equations present the stoichiometric description of the photosynthetic process assuming ammonium (Equation 1-36a) or nitrate (Equation 1-36b) as the nitrogen source and assuming algal biomass to have Redfield stoichiometry:

TABLE 1-8. SILICA REACTION EQUATIONS

Biogenic Silica (BSi)

$$S_{16} = \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_c - k_{16,17}\,\theta_{16,17}{}^{T-20} \cdot BSi \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{V_{s16}}{H} \cdot BSi$$

Available Silica (Si)

$$S_{17} = k_{16,17}\,\theta_{16,17}{}^{T-20} \cdot BSi \cdot \frac{P_c}{K_{mP_c} + P_c} - \left(1 - f_{ExPP}\right) \cdot a_{sc} \cdot G_P \cdot P_c$$

Description	Notation	Value	Units
Phytoplankton Biomass	P_c	—	mgC/L
Temperature Corrected Algal Respiration Rate	$k_{PR}(T)$	Eq. 1-11a	day^{-1}
Temperature Corrected Grazing Rate	$k_{grz}(T)$	Eq. 1-13	day^{-1}
Specific Phytoplankton Growth Rate	G_p	Eq. 1-5	day^{-1}
Silica to Carbon Ration	a_{sc}	Table 1-2	mgSi/mgC
Fraction of Primary Productivity Going to the Algal Exudate pool	f_{ExPP}	0.1	
Mineralization Rate of Biogenic Silica	$k_{16,17}$	0.1-0.25	day^{-1}
Temperature Coefficient	$\theta_{16,17}$	1.08	
Silica Settling Rate	V_{s16}	0.5-1.0	m/day

$$\text{Biomass} = C_{106}\ H_{263}\ O_{110}\ N_{16}\ P_{1} \tag{1-37}$$

Oxygen-deficient or under-saturated waters are replenished via atmospheric reaeration. The reaeration coefficient is a function of the average tidal velocity, wind and temperature, and is computed using Equations 1-38a and 1-38b:

$$\underset{\text{wind}}{k_a\ (20^{o}C) = K_L / H} \tag{1-38a}$$

$$\underset{\text{temperature}}{k_a\ (T) = k_a\ (20^{o}C)\,\theta_a^{T-20}} \tag{1-38b}$$

where

k_a = the surface mass transfer coefficient (m/day),

H = depth (m),

θ_a = temperature coefficient.

Dissolved oxygen saturation is a function of both temperature and salinity and is determined via Equation 1-39 (Standard Methods, 1992):

$$\begin{aligned} DO_{sat} = \exp\ [&-139.34411 + 1.575701 \cdot 10^{5} / T \\ &-6.642308 \cdot 10^{7} / T^{2} + 1.243800 \cdot 10^{10} / T^{3} \\ &-8.621949 \cdot 10^{11} / T^{4} - S(1.7674 \cdot 10^{-2} \\ &-10.754 / T + 2140.7 / T^{2})] \end{aligned} \tag{1-39}$$

where

S = salinity (psu),

T = temperature (°K).

Dissolved oxygen is diminished in the water column as a result of algal respiration, which is the reverse process of photosynthesis; as a result of nitrification:

$$NH_4^{+} + 2O_2 \Rightarrow NO_3^{-} + H_2O + 2H^{+} \tag{1-40}$$

as a result of the oxidation of carbonaceous material (including detrital phytoplankton):

$$CH_2O + O_2 \Rightarrow CO_2 + H_2O \tag{1-41}$$

and, if dissolved oxygen concentrations are sufficiently low, as a result of denitrification:

$$5CH_2O + 4NO_3^- + \Rightarrow 5CO_2 + 2N_2 + 7H_2O \tag{1-42}$$

Table 1-9 presents a summary of the dissolved oxygen mass balance equation and associated coefficients incorporated in the integrated eutrophication model.

TABLE 1-9. DISSOLVED OXYGEN AND O_2^* REACTION RATES

Sulfide Oxygen Equivalents (O_2^*)

$$S_{24} = K_{O_2^*}\ \theta_{O_2^*}{}^{T-20} \cdot O_2^* \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO_{O_2^*}} + DO}$$

Dissolved Oxygen (DO)

$$\begin{aligned}
S_{25} = {} & a_{OC} \cdot \alpha_{NH_4} \cdot G_P \cdot P_c + \left(a_{NO_3}c\right) \cdot \left(1 - \alpha_{NH_4}\right) \cdot G_P \cdot P_c \\
& + k_a \theta_a{}^{T-20} \cdot \left(DO_{sat} - DO\right) - a_{OC} \cdot k_{PR}\ (T) \cdot P_c \\
& - 2 \cdot a_{ON} \cdot k_{14,15} \theta_{14,15}{}^{T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO} \\
& - a_{OC} \cdot \Big[k_{20,0}\ \theta_{20,0}^{T-20} \cdot RDOC + k_{21,0}\ \theta_{21,0}^{T-20} \cdot LDOC \cdot \frac{LDOC}{K_{m_{LDOC}} + LDOC} \\
& + k_{22,0}\ \theta_{22,0}^{T-20} \cdot Re\,DOC \cdot \frac{Re\,DOC}{K_{mLDOC} + Re\,DOC} \\
& + k_{23,0}\ \theta_{23,0}^{T-20} \cdot ExDOC \cdot \frac{ExDOC}{K_{mLDOC} + ExDOC} \Big] \cdot \frac{P_c}{K_{mPc} + P_c} \cdot \frac{DO}{K_{DO} + DO} \\
& - k_{o_2^*} \theta_{o_2^*}{}^{T-20} \cdot O_2^* \cdot \frac{P_c}{K_{mPc} + P_c} \cdot \frac{DO}{K_{DO_{O_2^*}} + DO}
\end{aligned}$$

TABLE 1-9. DISSOLVED OXYGEN AND O_2^* REACTION RATES
(continued)

Rate Constants

Description	Notation	Value	Units
Oxygen to Carbon Ratio	a_{OC}	32/12	$mgO_2/mg\ C$
Oxygen to Nitrogen Ratio	a_{ON}	32/14	$mgO_2/mg\ N$
Oxygen to Carbon Ratio for Nitrate Uptake	α_{NO_3C}	$\frac{48}{14} a_{NC}$	$mgO_2/mg\ C$
Reaeration Rate at 20°C	k_a	Eq. 1.19a	day^{-1}
Temperature Coefficient	θ_a	1.024	none
Oxygen Transfer Coefficient	k_L	0.75-1.8	m/day
Dissolved Oxygen Saturation	DO_{sat}	Eq. 1.20	mgO_2/L
Oxidation Rates and Temperature Coefficients			
for RDOC	$k_{20,0}$ $\theta_{20,0}$	0.008-0.01 1.08	day^{-1}
for LDOC	$k_{21,0}$ $\theta_{21,0}$	0.10-0.15 1.047	day^{-1}
for ReDOC	$k_{22,0}$ $\theta_{22,0}$	0.25-0.3 1.047	day^{-1}
for ExDOC	$k_{23,0}$ $\theta_{23,0}$	0.1-0.125 1.08	day^{-1}
Oxidation Rate of Dissolved Sulfide	$k_{o_2^*}$	0.15-0.5	day^{-1}
Temperature Coefficient	$\theta_{o_2^*}$	1.08	
Half Saturation for Oxygen Limitation	$k_{DO_{o_2^*}}$	0.2	mgO_2/L

1.2.4 Specification of Input Variables Associated with the Eutrophication Model

As described earlier, the user has the choice of two algal growth formulation - the standard formulation and the Laws-Chalup formulation. The user can also select whether to simulate one, two, or three algal groups. In addition, the user can select from various options to specify the reaeration coefficient and the extinction coefficient. These selections are provided for via the first three constants specified in Card Group L (more specifically in L10). These constants are described below.

Constant Number	Name	Description
1	AGOPT	algal growth model option = 0, use standard or traditional algal growth kinetics = 1, use Laws-Chalup formulation
2	ACTALG	number of algal groups to simulate = 1, just one group (state-variable #2) will be simulated = 2, two groups will be simulated (using state-variables #2 and #3) = 3, three algal groups will be simulated (using state-variables #2 through #4)
3	KAOPT	reaeration formulation option = 0, use spatially constant k_L ($k_a = k_L/\text{depth}$) = 1, use spatially variable k_L = 2, use velocity shear and oxygen diffusivity = 3, use wind shear formulation
4	KEOPT	extinction coefficient option = 0, k_e is a constant (spatially and temporally invariant = 1, k_e is a spatially variable but constant in time(using 2-d parameter array) = 2, k_e is spatially invariant but varies in time (using time-variable function) = 3, k_e is spatially variable and can vary in time, (using 2-d parameter array and one time-variable function) = 4, k_e is spatially and temporally variable (requires separate input file)

TABLE 1-10. KINETIC CONSTANTS USED FOR STANDARD EUTROPHICATION ALGAL GROWTH MODEL

If <AGOPT> = 0 then the following constants (9 through 99) are used by the eutrophication model and must be specified by the user. If the user is simulating only one phytoplankton group then constants 41-99 can be ignored; if the user is simulating two group then constants 73-99 can be ignored.

Number	Name	Description	Units
9	TOPT1	optimal growth temperature for algal group #1	deg C
10	K1BETA1	temperature correction effect on growth rate below <TOPT1>	(deg C)$^{-2}$
11	K1BETA2	temperature correction effect on growth rate above <TOPT1>	(deg C)$^{-2}$
12	K1C	saturated phytoplankton growth rate (at temperature = <TOPT1>)	/day
13	K1T	temperature coefficient	
14	IS1	saturating algal light intensity	ly/day
15	KMN1	half saturation constant for nitrogen	mg N/L
16	KMP1	half saturation constant for phosphorous	mg P/L
17	KMS1	half saturation constant for silica	mg Si/L
18	K1RB	basal/resting respiration rate -or- endogenous respiration rate at 20 deg C	/day
19	K1RT	temperature coefficient	
20	K1RG	growth-rate-dependent respiration coefficient	
21	K1GRZC	death rate due to grazing	/day
22	K1GRZT	temperature coefficient	
23	CCHL1	carbon to chlorophyll ratio	mg C/mg Chla
24	CRBP11	carbon to phosphorus ratio - non-P limited	mg C/mg P
25	CRBP12	carbon to phosphorus ratio - P limited	mg C/mg P
26	CRBP13	coefficient determining range of P limitation	L/mg P
27	CRBN11	carbon to nitrogen ratio - non-N limited	mg C/mg N
28	CRBN12	carbon to nitrogen ratio - N limited	mg C/mg N
29	CRBN13	coefficient determining range of N limitation	L/mg N
30	CRBS11	carbon to silica ratio - non-Si limited	mg C/mg Si
31	CRBS12	carbon to silica ratio - Si limited	mg C/mg Si
32	CRBS13	coefficient determining range of Si limitation	L/mg Si
33	XKC1	chlorophyll self-shading extinction coefficient	m^2/mg Chla
34	VSBAS1	base algal settling rate	m/day
35	VSNTR1	nutrient stressed algal settling rate	m/day

TABLE 1-10. KINETIC CONSTANTS USED FOR STANDARD EUTROPHICATION ALGAL GROWTH MODEL (Continued)

41	TOPT2	optimal growth temperature for algal group #2	deg C
42	K2BETA1	temperature correction effect on growth rate below <TOPT2>	(deg C)$^{-2}$
43	K2BETA2	temperature correction effect on growth rate above <TOPT2>	(deg C)$^{-2}$
44	K2C	saturated phytoplankton growth rate (at temperature = <TOPT2>)	/day
45	K2T	temperature coefficient	
46	IS2	saturating algal light intensity	ly/day
47	KMN2	half saturation constant for nitrogen	mg N/L
48	KMP2	half saturation constant for phosphorous	mg P/L
49	KMS2	half saturation constant for silica	mg Si/L
50	K2RB	basal/resting respiration rate -or- endogenous respiration rate at 20 deg C	/day /day
51	K2RT	temperature coefficient	
52	K2RG	growth-rate-dependent respiration coefficient	
53	K2GRZC	death rate due to grazing	/day
54	K2GRZT	temperature coefficient	
55	CCHL2	carbon to chlorophyll ratio	mg C/mg Chla
56	CRBP21	carbon to phosphorus ratio - non-P limited	mg C/mg P
57	CRBP22	carbon to phosphorus ratio - P limited	mg C/mg P
58	CRBP23	coefficient determining range of P limitation	L/mg P
59	CRBN21	carbon to nitrogen ratio - non-N limited	mg C/mg N
60	CRBN22	carbon to nitrogen ratio - N limited	mg C/mg N
61	CRBN23	coefficient determining range of N limitation	L/mg N
62	CRBS21	carbon to silica ratio - non-Si limited	mg C/mg Si
63	CRBS22	carbon to silica ratio - Si limited	mg C/mg Si
64	CRBS23	coefficient determining range of Si limitation	L/mg Si
65	XKC2	chlorophyll self-shading extinction coefficient	m^2/mg Chla
66	VSBAS2	base algal settling rate	m/day
67	VSNTR2	nutrient stressed algal settling rate	m/day

TABLE 1-10. KINETIC CONSTANTS USED FOR STANDARD EUTROPHICATION ALGAL GROWTH MODEL (Continued)

73	TOPT3	optimal growth temperature for algal group #3	deg C
74	K3BETA1	temperature correction effect on growth rate below <TOPT1>	$(\text{deg C})^{-2}$
75	K3BETA2	temperature correction effect on growth rate above <TOPT1>	$(\text{deg C})^{-2}$
76	K3C	saturated phytoplankton growth rate (at temperature = <TOPT1>)	/day
77	K3T	temperature coefficient	
78	IS3	saturating algal light intensity	ly/day
79	KMN3	half saturation constant for nitrogen	mg N/L
80	KMP3	half saturation constant for phosphorous	mg P/L
81	KMS3	half saturation constant for silica	mg Si/L
82	K1RB	basal/resting respiration rate -or- endogenous respiration rate at 20 deg C	/day /day
83	K3RT	temperature coefficient	
84	K3RG	growth-rate-dependent respiration coefficient	
85	K3GRZC	death rate due to grazing	/day
86	K3GRZT	temperature coefficient	
87	CCHL3	carbon to chlorophyll ratio	mg C/mg Chla
88	CRBP31	carbon to phosphorus ratio - non-P limited	mg C/mg P
89	CRBP32	carbon to phosphorus ratio - P limited	mg C/mg P
90	CRBP33	coefficient determining range of P limitation	L/mg P
91	CRBN31	carbon to nitrogen ratio - non-N limited	mg C/mg N
92	CRBN32	carbon to nitrogen ratio - N limited	mg C/mg N
93	CRBN33	coefficient determining range of N limitation	L/mg N
94	CRBS31	carbon to silica ratio - non-Si limited	mg C/mg Si
95	CRBS32	carbon to silica ratio - Si limited	mg C/mg Si
96	CRBS33	coefficient determining range of Si limitation	L/mg Si
97	XKC3	chlorophyll self-shading extinction coefficient	m^2/mg Chla
98	VSBAS3	base algal settling rate	m/day
99	VSNTR3	nutrient stressed algal settling rate	m/day
105	KMPHYT	half saturation constant for phytoplankton	mg C/L

TABLE 1-11. KINETIC CONSTANTS USED FOR LAWS-CHALUP EUTROPHICATION ALGAL GROWTH MODEL

If <AGOPT> = 1 then the following constants (6 through 95) are used by the eutrophication model and must be specified by the user. If the user is simulating only one phytoplankton group, then constants 41-95 can be ignored; if the user is simulating only two groups, then constants 73-95 can be ignored.

9	TOPT1	optimal growth temperature for algal group #1	deg C
10	K1BETA1	temperature correction effect on growth rate below <TOPT1>	$(\text{deg C})^{-2}$
11	K1BETA2	temperature correction effect on growth rate above <TOPT1>	$(\text{deg C})^{-2}$
12	GPRE1	gross photosynthetic rate per unit cell (associated with photosynthetic dark reactions)	/day
13	GPR01	gross photosynthetic rate per unit cell per unit light intensity under nutrient-saturated conditions and zero irradiance	m^2/mol quanta
14	IS1	saturating algal light intensity	ly/day
15	KMN1	half saturation constant for nitrogen	mg N/L
16	KMP1	half saturation constant for phosphorous	mg P/L
17	KMS1	half saturation constant for silica	mg Si/L
18	K1RB	basal or resting respiration rate	/day
19	K1RT	temperature coefficient for basal/endogenous respiration	
20	K1RG	growth-rate-dependent respiration coefficient	
21	K1GRZC	death rate due to grazing	/day
22	K1GRZT	temperature coefficient	
23	FSC1	fraction of C allocated to structural purposes	
24	WCCHL1	carbon to chlorophyll ratio	mg C/mg Chla
25	WCP1	carbon to phosphorus ratio - non-P limited	mg C/mg P
26	WCN1	carbon to nitrogen ratio - non-N limited	mg C/mg N
27	WCS1	carbon to silica ratio - non-Si limited	mg C/mg Si
28	QF1	quotient of nutrient-limited nutrient:C ratios at relative growth rates of 0 and 1	
29	XKC1	chlorophyll self-shading extinction coefficient	m^2/mg Chla
30	VSBAS1	base algal settling rate	m/day
31	VSNTR1	nutrient stressed algal settling rate	m/day

TABLE 1-11. KINETIC CONSTANTS USED FOR LAWS-CHALUP EUTROPHICATION ALGAL GROWTH MODEL (Continued)

41	TOPT2	optimal growth temperature for algal group #2	deg C
42	K2BETA1	temperature correction effect on growth rate below <TOPT2>	(deg C)$^{-2}$
43	K2BETA2	temperature correction effect on growth rate above <TOPT2>	(deg C)$^{-2}$
44	GPRE2	gross photosynthetic rate per unit cell (associated with photosynthetic dark reactions)	/day
45	GPR02	gross photosynthetic rate per unit cell per unit light intensity under nutrient-saturated conditions and zero irradiance	m^2/mol quanta
46	IS2	saturating algal light intensity	ly/day
47	KMN2	half saturation constant for nitrogen	mg N/L
48	KMP2	half saturation constant for phosphorous	mg P/L
49	KMS2	half saturation constant for silica	mg Si/L
50	K2RB	basal or resting respiration rate	/day
51	K2RT	temperature coefficient for basal/endogenous respiration	
52	K2RG	growth-rate-dependent respiration coefficient	
53	K2GRZC	death rate due to grazing	/day
54	K2GRZT	temperature coefficient	
55	FSC2	fraction of C allocated to structural purposes	
56	WCCHL2	carbon to chlorophyll ratio	mg C/mg Chla
57	WCP2	carbon to phosphorus ratio - non-P limited	mg C/mg P
58	WCN2	carbon to nitrogen ratio - non-N limited	mg C/mg N
59	WCS2	carbon to silica ratio - non-Si limited	mg C/mg Si
60	QF2	quotient of nutrient-limited nutrient: C ratios at relative growth rates of 0 and 1	
61	XKC2	chlorophyll self-shading extinction coefficient	m^2/mg Chla
62	VSBAS2	base algal settling rate	m/day
63	VSNTR2	nutrient stressed algal settling rate	m/day

TABLE 1-11. KINETIC CONSTANTS USED FOR LAWS-CHALUP EUTROPHICATION ALGAL GROWTH MODEL (Continued)

73	TOPT3	optimal growth temperature for algal group #3	deg C
74	K3BETA1	temperature correction effect on growth rate below <TOPT1>	(deg C)$^{-2}$
75	K3BETA2	temperature correction effect on growth rate above <TOPT1>	(deg C)$^{-2}$
76	GPRE3	gross photosynthetic rate per unit cell (associated with photosynthetic dark reactions)	/day
77	GPR03	gross photosynthetic rate per unit cell per unit light intensity under nutrient-saturated conditions and zero irradiance	m^2/mol quanta
78	IS3	saturating algal light intensity	ly/day
79	KMN3	half saturation constant for nitrogen	mg N/L
80	KMP3	half saturation constant for phosphorous	mg P/L
81	KMS3	half saturation constant for silica	mg Si/L
82	K3RB	basal or resting respiration rate	/day
83	K3RT	temperature coefficient for basal/endogenous	
84	K3RG	growth-rate-dependent respiration coefficient respiration	
85	K3GRZC	death rate due to grazing	/day
86	K3GRZT	temperature coefficient	
87	FSC3	fraction of C allocated to structural purposes	
88	WCCHL3	carbon to chlorophyll ratio	mg C/mg Chla
89	WCP3	carbon to phosphorus ratio - non-P limited	mg C/mg P
90	WCN3	carbon to nitrogen ratio - non-N limited	mg C/mg N
91	WCS3	carbon to silica ratio - non-Si limited	mg C/mg Si
92	QF3	quotient of nutrient-limited nutrient: C ratios at relative growth rates of 0 and 1	
93	XKC3	chlorophyll self-shading extinction coefficient	m^2/mg Chla
94	VSBAS3	base algal settling rate	m/day
95	VSNWTR3	nutrient stressed algal settling rate	m/day
105	KMPHYT	half saturation constant for phytoplankton	mg C/L

TABLE 1-12. REMAINING KINETIC CONSTANTS USED FOR INTEGRATED EUTROPHICATION MODEL

		Recycle Fractions - Fraction of Grayed/Respired Algal Biomass Going to....	
106	FRPOP	refractory particulate organic phosphorous	
107	FLPOP	labile particulate organic phosphorous	
108	FRDOP	refractory dissolved organic phosphorous	
109	FLDOP	labile dissolved organic phosphorous	
110	FPO4	dissolved inorganic phosphorous	
111	FRPON	refractory particulate organic nitrogen	
112	FLPON	labile particulate organic nitrogen	
113	FRDON	refractory dissolved organic nitrogen	
114	FLDON	labile dissolved organic nitrogen	
115	FNH4	ammonia	
116	FRPOC	refractory particulate organic carbon	
117	FLPOC	labile particulate organic carbon	
118	FRDOC	refractory dissolved organic carbon	
119	FLDOC	labile dissolved organic carbon	
		Phosphorus Hydrolysis/Mineralization Rates at 20 deg C	
120	K57C	hydrolysis rate of RPOP to RDOP	/day
121	K57T	temperature coefficient	
122	K68C	hydrolysis rate of LPOP to LDOP	/day
123	K68T	temperature coefficient	
124	K79C	mineralization rate of RDOP to PO4	/day
125	K79T	temperature coefficient	
126	K89C	mineralization rate of LDOP to PO4	/day
127	K89T	temperature coefficient	
		Nitrogen Hydrolysis/Mineralization Rates at 20 deg C	
128	K1012C	hydrolysis rate of RPON to RDON	/day
129	K1012T	temperature coefficient	
130	K1113C	hydrolysis rate of LPON to LDON	/day
131	K1113T	temperature coefficient	
132	K1214C	mineralization rate of RDON to NH4	/day
133	K1214T	temperature coefficient	
134	K1314C	mineralization rate of LDON to NH4	/day
135	K1314T	temperature coefficient	

TABLE 1-12. REMAINING KINETIC CONSTANTS USED FOR INTEGRATED EUTROPHICATION MODEL (Continued)

		Nitrification/Denitrification Rates	
136	K1415C	nitrification rate at 20 deg C	/day
137	K1415T	temperature coefficient	
138	KNIT	half saturation constant for nitrification oxygen limitation	mg O2/L
139	K150C	denitrification rate at 20 deg C	/day
140	K150T	temperature coefficient	
141	KNO3	Michaelis constant for denitrification oxygen limitation	mg O2/L
		Silica Mineralization Rates at 20 deg C	
142	K1617C	mineralization rate of biogenic Si to available dissolved Si	/day
143	K1617T	temperature coefficient	
		Carbon Hydrolysis/Oxidation Rates at 20 deg C	
144	K1820C	hydrolysis rate of RPOC to RDOC	/day
145	K1820T	temperature coefficient	
146	K1921C	hydrolysis rate of LPOC to LDOC	/day
147	K1921T	temperature coefficient	
148	K200C	oxidation rate of RDOC	/day
149	K200T	temperature coefficient	
150	K210C	oxidation rate of LDOC	/day
151	K210T	temperature coefficient	
152	KMLDOC	Michaelis constant for LDOC	mg C/L
153	KDOC	half saturation constant for organic carbon	mg O2/L
154	K220C	algal exudate DOC oxidation rate	/day
155	K220T	temperature coefficient	
156	FLOCEX	fraction of primary productivity going to labile organic carbon via exudation	
157	K2324C	hydrolysis rate of REPOC to REDOC	/day
158	K2324T	temperature coefficient	
159	K240C	reactive DOC oxidation rate	/day
160	K240T	temperature coefficient	
161	CTOPCSO	carbon to phosphorus ratio of CSO solids	mg C/mg P
162	CTONCSO	carbon to nitrogen ratio of CSO solids	mg C/mg N
163	K250C	oxidation rate for aqueous sod	/day
164	K250T	temperature coefficient	

TABLE 1-12. REMAINING KINETIC CONSTANTS USED FOR INTEGRATED EUTROPHICATION MODEL (Continued)

165	KO2EQ	half saturation constant for O_2^*	mg O_2/L
166	KLMIN	if <KAOPT> = 0, then $K_{lmin} = K_l$ if <KAOPT> > 0, then K_{lmin} = minimum value for K_l	m/day
167	DIFUS	diffusivity of oxygen across the air-water interface	m^2/day
168	KAT	temperature correction coefficient for atmospheric reaeration	
169	VSBAST	temperature correction	
170	VSPOM	particulate organic matter settling rate	m/day
171	VSPMT	temperature correction	
172	VSSEDT	temperature correction for deposition to sediment	
173	BVCSO	power coefficient for CSO solid settling rate (>=1)	unitless
174	CRCSO	critical REPOC concentration for CSO settling function	mg C/L
175	VMINCSO	minimum settling rate for CSO solids Vcso =min (VMAXCSO + VMINCSO + (VMAXCSO - VMINCSO) * (REPOC/CRCSO)**BVCSO)	m/day
176	VMAXCSO	maximum settling rate for CSO solids	m/day
177	KADPO4	partition coefficient for sorbed phosphorus	L/mg ss
178	KADSI	partition coefficient for sorbed silica	L/mg ss
179	VSPIM	settling rate for phosphorus/silica sorbed to suspended solids	m/day
180	KECONST	base (chl-a corrected) extinction coefficient (used when <KEOPT> = 0,2)	/m

1.2.4.1 Parameters, Constants, and Time Functions

The parameters, constants, and time functions required by the kinetics of this model are specified according to the formatting described for input Group L in the RCA Users Guide. Table 1-13 lists the required two dimensional segment parameters. No three dimensional parameters are included in the kinetic routine. Required time variable functions are described in Table 1-14.

TABLE 1-13. 2-D PARAMETERS

Number	Name	Description	Units
1	KL	transfer coefficient for reaeration	m/day
2	VSNET1	settling efficiency from water column to the bed for algal group number 1 (the winter diatom group)	
3	VSNET2	settling efficiency from water column to the bed for algal group number 2 (the summer mixed assemblage)	m/day
4	VSNET3	settling efficiency from water column to bed for algal group number 3	m/day
5	VSNET4	settling efficiency from water column to the bed for non-living particulate organic matter (POM)	m/day
6	KEBS	base extinction coefficient (when KEOPT - 1 or 3)	m^{-1}

Note: by settling efficiency, it is meant the "stickiness" of a particle settling from the water column to the sediment bed; range 0 to 1. If VSNET = 1, all of the particles settling from the water column to the bed, stick to the bed and become incorporated in the sediment. If VSNET = 0.5, only half of the particles settling from the water column to the bed become incorporated in the sediment; the remainder are assumed to become "resuspended" and may be transported elsewhere. If VSNET = 0, none of the particles settle to the bed, i.e., no deposition in this segment.

TABLE 1-14. TIME-VARIABLE FUNCTIONS

Number	Name	Description	Units
1	ITOTSF	total daily solar radiation	ly/day
2	F	fraction of daylight	day
3	WIND	wind speed	m/sec
4	KETVF	extinction coefficient (when KEOPT = 2 or 3)	m^{-1}

Table 1-15 presents a sample input deck for the standard eutrophication model coefficient set, which includes one kinetic subroutine specific file, i.e., the sediment nutrient flux subroutine input data set.

TABLE 1-15. SAMPLE EUTROPHICATION INPUT DATASET

```
C N2DPARAM
         6
C   Scale1    Scale2    Scale3    Scale4
    0.3048       1.0       1.0       1.0
kL
    0.0000    0.0000    0.0000
    0.0000    0.7870    0.0000
    0.0000    0.0000    0.0000
Vsnet1 - algal group 1
    0.0000    0.0000    0.0000
    0.0000    1.0000    0.0000
    0.0000    0.0000    0.0000
Vsnet2 - algal group 2
    0.0000    0.0000    0.0000
    0.0000    1.0000    0.0000
    0.0000    0.0000    0.0000
Vsnet3 - algal group 3
    0.0000    0.0000    0.0000
    0.0000    1.0000    0.0000
    0.0000    0.0000    0.0000
Vsnet4 - pom
    0.0000    0.0000    0.0000
    0.0000    1.0000    0.0000
    0.0000    0.0000    0.0000
KEbs
    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000
C N3DPARAM
    1                                    number of 3D parameters
C   SCALE1
   1.0E-20
SS (mg/L)
      0.01      0.01      0.01
      0.01      0.01      0.01
      0.01      0.01      0.01           Layer #1
      0.01      0.01      0.01
      0.01      0.01      0.01
      0.01      0.01      0.01           Layer #2
C    NCONS
       180                                   number of constants
     AGOPT    ACTALG     KAOPT     KEOPT    Unused    Unused    Unused    Unused
        0.        2.        1.        2.
     TOPT1   K1BETA1   K2BETA2       K1C       K1T       IS1      KMN1      KMP1
      3.50      .004      .006     2.500     1.068   150.000     0.010     0.001
      KMS1      K1RB      K1RT      K1RG     K1GZC     K1GZT     CCHL1     CPR11
     0.020     0.075     1.047       0.0     0.100      1.10      30.0      40.0
     CPR12     CPR13     CNR11     CNR12     CNR13     CSR11     CSR12     CSR13
       0.0       0.0     5.670       0.0       0.0       5.0      10.0       0.0
      XKC1    VSBAS1    VSNTR1    Unused    Unused    Unused    Unused    Unused
     0.017       0.2       0.5
     TOPT2   K2BETA1   K2BETA2       K2C       K2T       IS2      KMN2      KMP2
       22.      .004      .006     2.400     1.068     350.0     0.010     0.001
      KMS2      K2RB      K2RT      K2RG     K2GZC     K2GRT     CCHL2     CPR21
     0.002     0.075     1.047       0.0     0.120     1.100      80.0      40.0
     CPR22     CPR23     CNR21     CNR22     CNR23     CSR21     CSR22     CSR23
       0.0       0.0     5.670       0.0       0.0       8.0       0.0       0.0
      XKC2    VSBAS2    VSNTR2    Unused    Unused    Unused    Unused    Unused
     0.017       0.5       0.2
     TOPT3   K3BETA1   K3BETA2       K3C       K3T       IS3      KMN3      KMP3
        0.        0.        0.        0.        0.        0.        0.        0.
      KMS3      K3RB      K3RT      K3RG     K3GZC     K3GRT     CCHL3     CPR31
        0.        0.        0.        0.        0.        0.        0.        0.
     CPR32     CPR33     CNR31     CNR32     CNR33     CSR31     CSR32     CSR33
```

TABLE 1-15. SAMPLE EUTROPHICATION INPUT DATASET (Cont.)

```
        0.        0.        0.        0.        0.        0.        0.        0.
      XKC3    VSBAS3    VSNTR3    Unused    Unused    Unused    Unused    Unused
        0.        0.        0.
     KMPHY     FRPOP     FLPOP     FRDOP     FLDOP      FPO4     FRPON     FLPON
     0.050     0.100     0.250     0.100     0.100     0.450     0.001     0.399
     FRDON     FLDON      FNH4     FRPOC     FLPOC     FRDOC     FLDOC      K57C
     0.125     0.125     0.350     0.001     0.449     0.100     0.450     0.010
      K57T      K68C      K68T      K79C      K79T      K89C      K89T    K1012C
     1.080     0.070     1.080     0.020     1.080     0.090    1.080      0.010
    K1012T    K1113C    K1113T    K1214C    K1214T    K1314C    K1314T    K1415C
     1.080     0.050     1.080     0.010     1.080     0.075    1.080      0.040
    K1415T      KNIT     K150C     K150T      KNO3    K1617C    K1617T    K1820C
     1.040     1.500     0.050     1.045     0.010      0.10     1.080     0.010
    K1820T    K1921C    K1921T     K200C     K200T     K210C     K210T    KMLDOC
     1.080     0.070     1.080     0.010     1.080     0.150     1.047     0.100
      KDOC     K220C     K220T    FLOCEX    K2324C    K2324T     K240C     K240T
     0.200     0.120     1.047       0.0      0.35     1.047     0.100     1.080
   CTOPCSO   CTONCSO     K250C     K250T     KO2EQ     KLMIN     DIFUS       KAT
       35.       6.0     0.150     1.080     0.100       2.0      0.00     1.024
    VSBAST     VSPOM     VSPMT    VSSEDT     BVCSO     CRCSO    KADPO4     KADSI
     1.000     0.750      1.00       1.0       2.0       10.       6.0       6.0
     VSPIM   KECONST
       0.0       0.0
C    NOTVF  TVPWLOPT
        4          1                 number of time functions
C    PNAME     NOBRK  TWARPTVF
      ITOT        13      DAYS       TOTAL DAILY RADIATION
      118.        0.      168.       11.      218.       59.      318.       90.
      418.      120.      468.      151.      518.      181.      468.      212.
      418.      243.      318.      273.      218.      304.      168.      335.
      118.      365.
C    PNAME     NOBRK  TWARPTVF
     F DAY        13      DAYS       FRACTION OF DAYLIGHT
      0.37        0.      0.42       31.      0.46       59.      0.52       90.
      0.58      120.      0.61      151.      0.63      181.      0.59      212.
      0.54      243.      0.49      273.      0.43      304.      0.40      335.
      0.37      365.
C    PNAME     NOBRK  TWARPTVF
      Wind         2      DAYS       Wind Speed (m/sec)
      000.        0.      000.     9999.
C    PNAME     NOBRK  TWARPTVF
        KE        13      DAYS       Extinction coefficient (/m)
      0.70        0.      0.65       31.      0.60       59.      0.55       90.
      0.73      120.      0.96      151.      1.12      181.      0.74      212.
      0.57      243.      0.57      273.      0.51      304.      0.63      335.
      0.67      365.
C NOKINFIL                           Number of kinetic subroutine specific files
        1
sed.inp
```

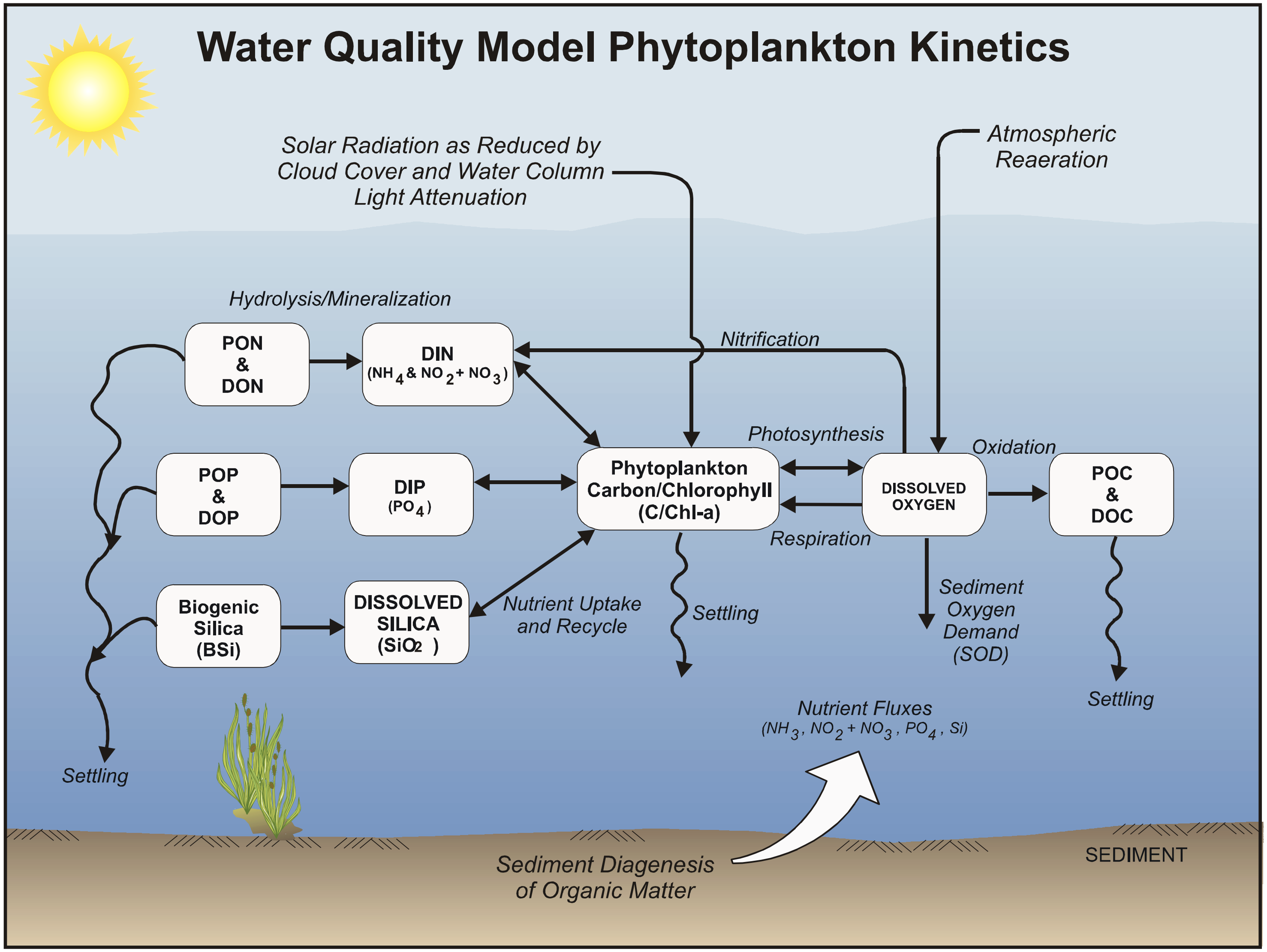


Figure 1-1. Principal Kinetic Interactions for Nutrient Cycles and Dissolved Oxygen

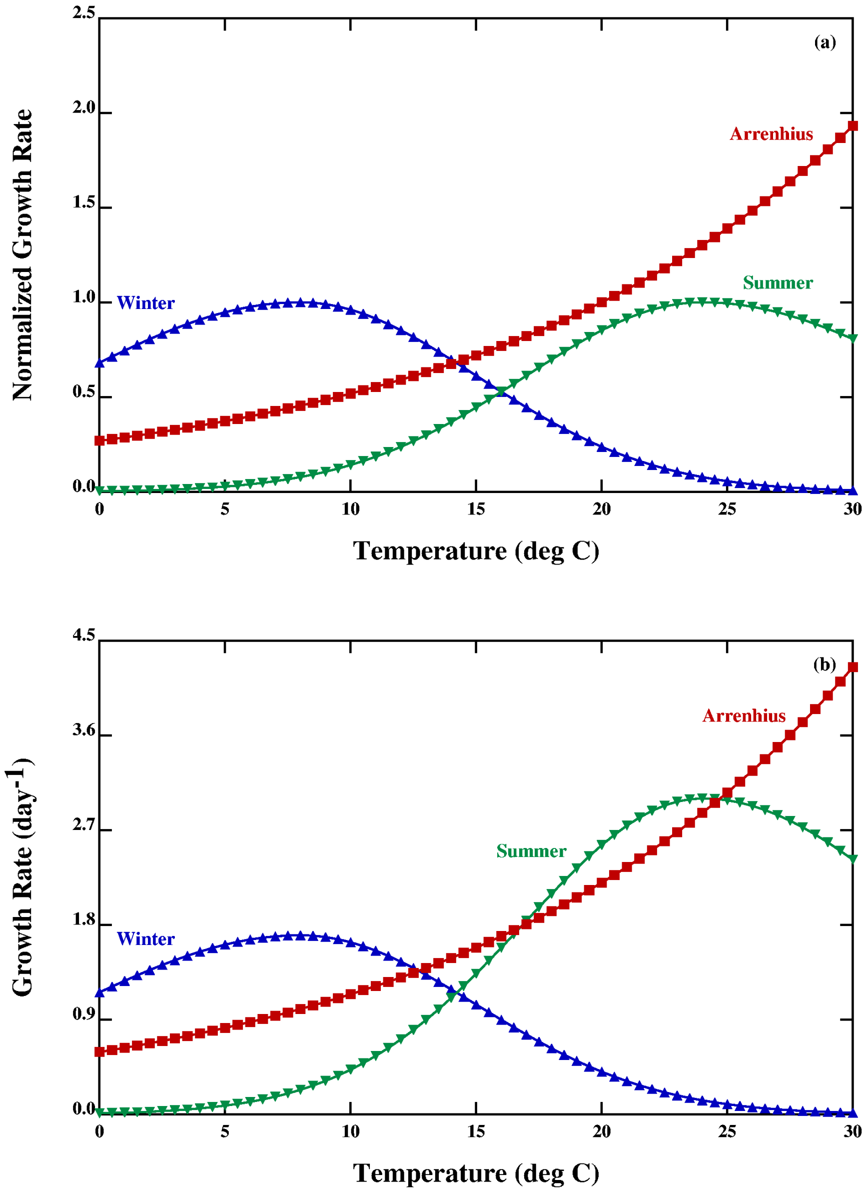


Figure 1-2. Growth Rate as a Function of Temperature

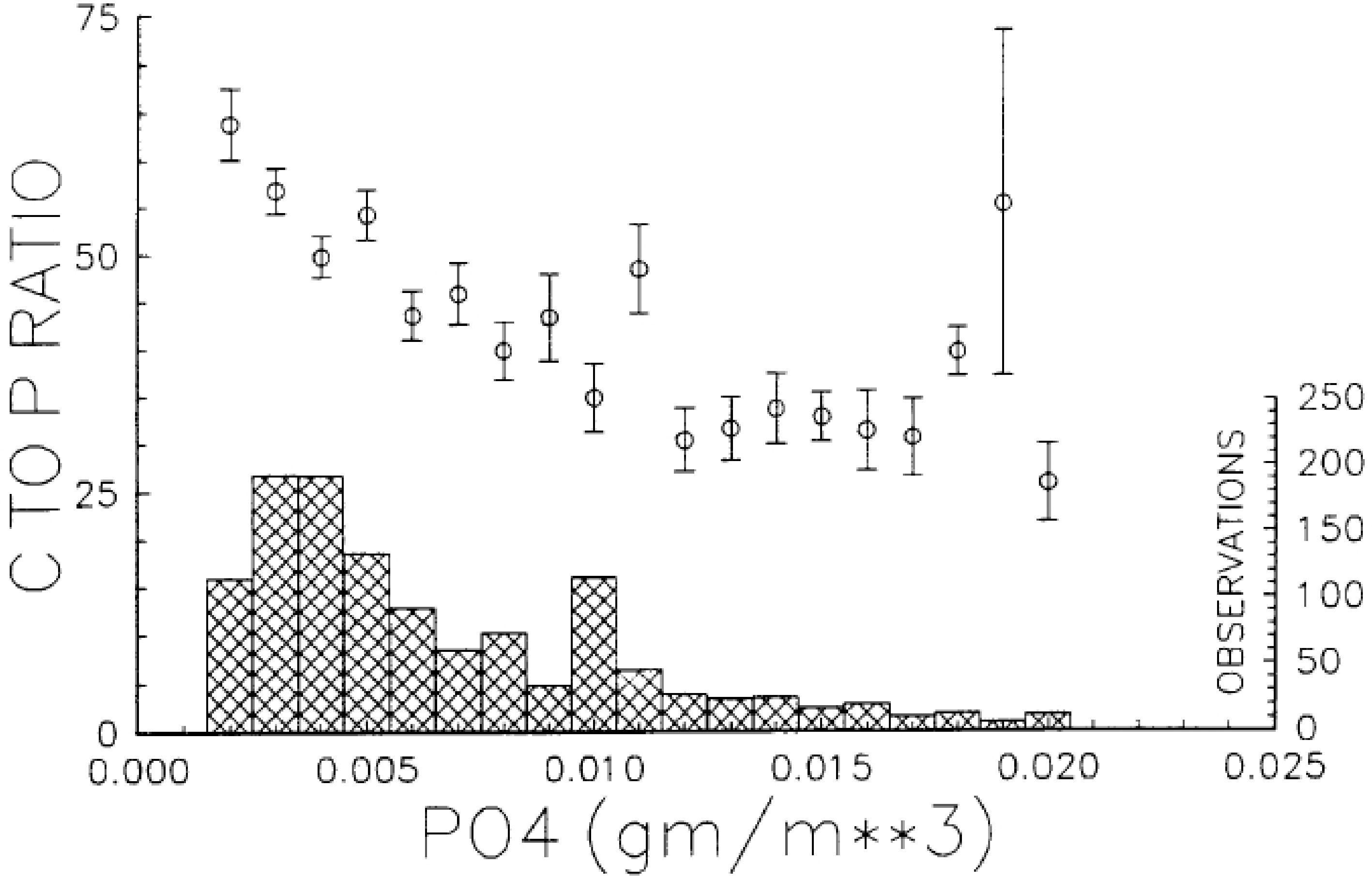


Figure 1-3. Carbon-to-phosphorus ratio (mean and standard error) of seston in Upper Chesapeake Bay. Bars show number of observations.

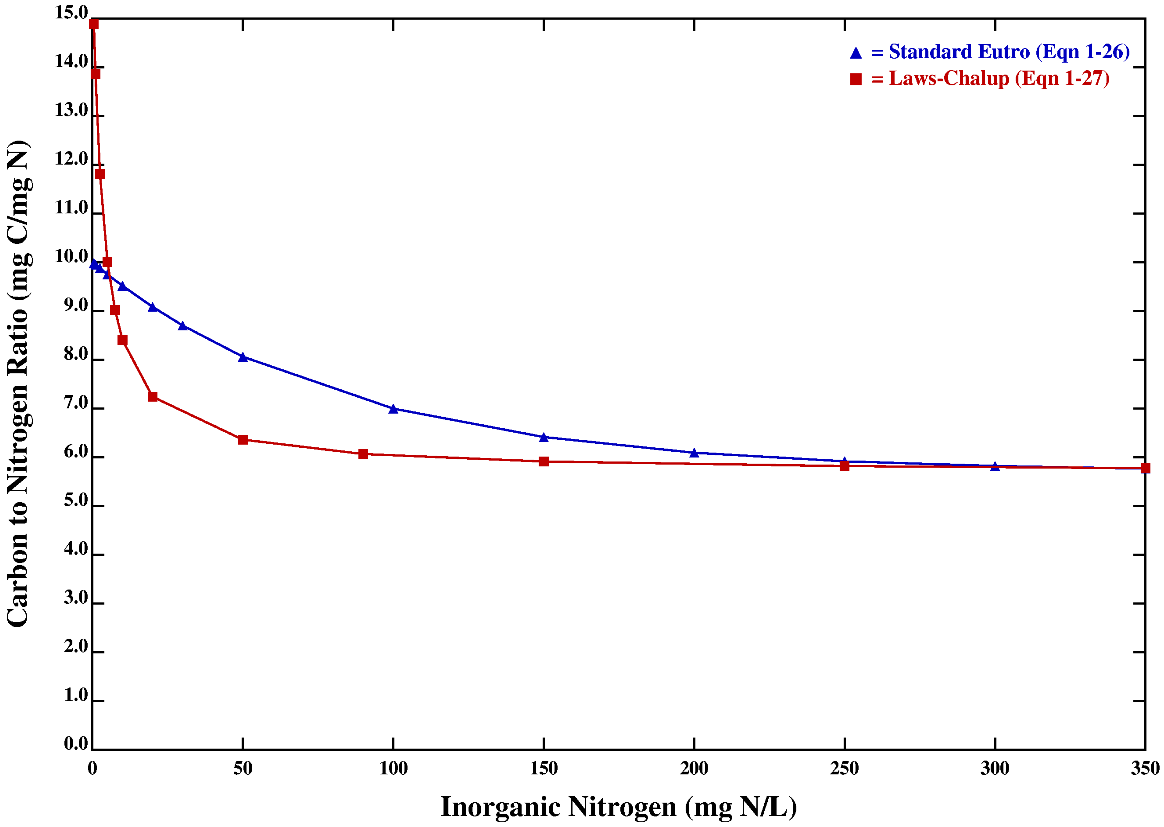


Figure 1-4. Carbon to nitrogen ratios as a function of the concentration of dissolved inorganic nitrogen.

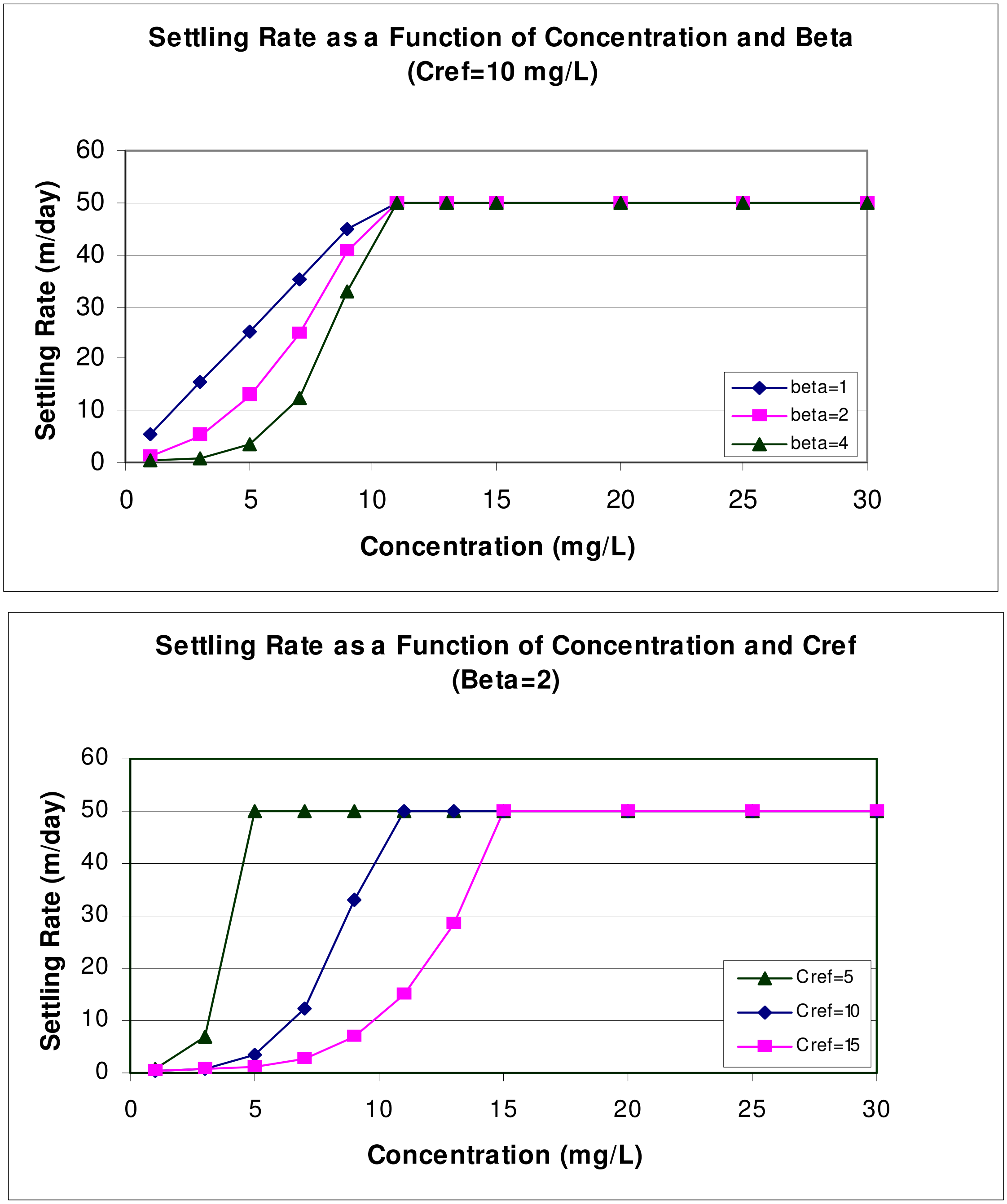


Figure 1-5. Settling Rate as a Function of Concentration and β (Beta) and C_{ref}

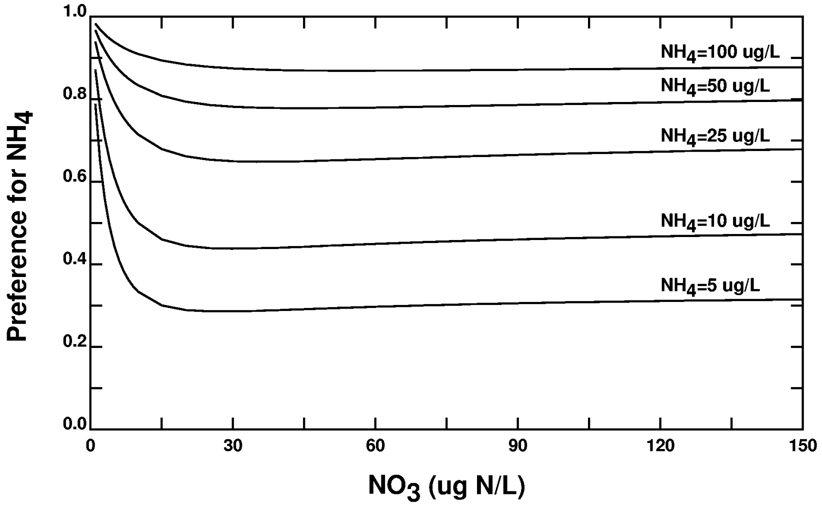


Figure 1-6. Behavior of the Ammonia Preference Structure for Various Concentrations of NH_3 and NO_2+NO_3.

2.0 FRAMEWORK FOR THE SEDIMENT FLUX SUBMODEL

2.1 Overview of Model Framework

The sediment receives fluxes of particulate organic carbon (POC), particulate organic nitrogen (PON), and particulate organic phosphorus (POP). This is collectively referred to as particulate organic matter (POM). Mineralization, which is termed diagenesis, produces soluble end-products. These can react in the aerobic and anaerobic layers of the sediment. The difference between the resulting aerobic layer dissolved concentration and the overlying water concentration determines the flux to or from the sediment. The magnitude of the flux is determined by the surface mass transfer coefficient.

2.2 Diagenesis

The water column model state-variables that are deposited to the sediment include: detrital algae, labile and refractory POC, labile and refractory PON, and labile and refractory POP. The fluxes of these state variables make up the incoming sources of particulate organic matter to the sediment. Carbon, nitrogen, and phosphorus are treated analogously.

The multi-class G model (Westrich and Berner 1984) is used as the basis for the diagenesis of POM. Each class represents a portion of the organic material that reacts at a specific rate. The reaction rates for each class are approximately an order of magnitude smaller than the previous class. For this application three G classes are chosen. The three classes represent three scales of reactivity: reactive (~20 day half life); refractory (~1 year half life); and inert (i.e., conservative). Particulate organic matter is also allowed to be removed by burial.

The kinetic equations for particulate organic carbon, nitrogen, and phosphorus are analogous. Let $G_{POC,i}$ be the concentration of POC in the ith diagenesis class (i=1, 2, or 3). The kinetic equation for diagenesis is:

$$H \frac{dG_{POC,i}}{dt} = - k_{GPOC,i} \, \theta_{GPOC,i}^{T-20} \, G_{POC,i} \, H + J_{GPOC,i}(t) \tag{2-1}$$

where:

H = depth of the active sediment layer [m],
$G_{POC,i}$ = concentration of particulate organic carbon in reactivity class i, (g/m^3)
$k_{GPOC,i}$ = first order reaction rate coefficient ($k_{GPOC,3} = 0$), (/day),

$\theta_{GPOC,i}$ = temperature coefficient,

$J_{GPOC,i}(t)$ = POC flux of the i^{th} G class to the sediment from the overlying water, (g/m^2-day).

The water column sources that contribute to each reactivity class are:

$J_{GPOC.1} = f_{G1} J_{POC}$

$J_{GPOC,2} = f_{G2} J_{POC}$

$J_{GPOC,3} = f_{G3} J_{POC}$

where:

f_{G1} = fraction of water column POC that is in reactivity class G_1

f_{G2} = fraction of water column POC that is in reactivity class G_2

f_{G3} = fraction of water column POC that is in reactivity class G_3

J_{POC} = total flux of POC from the overlying water column to the sediment bed

Carbon diagenesis flux, J_C, is computed from the rates of mineralization of the labile and refractory G classes. (Note: it is assumed that G_3 carbon is inert; therefore, it does not contribute to carbon diagenesis):

$$J_C = \sum_{i=1}^{2} k_{GPOC,i}\ \theta_{GPOC,i}^{(T-20)}\ G_{POC,i}\ H \qquad (2\text{-}2)$$

Nitrogen and phosphorus are completely analogous.

$$J_N = \sum_{i=1}^{2} k_{GPON,i}\ \theta_{GPON,i}^{(T-20)}\ G_{PON,i}\ H \qquad (2\text{-}3)$$

$$J_P = \sum_{i=1}^{2} k_{GPOP,i}\ \theta_{GPOP,i}^{(T-20)}\ G_{POP,i}\ H \qquad (2\text{-}4)$$

The reaction rates and temperature coefficients are analogous to those listed above for carbon.

2.3 The General Sediment Model Equations

The sediment model is constructed from a mass balance equation in the aerobic layer, denoted as layer 1, and the anaerobic layer, layer 2 (with the overlying water column concentrations denoted using the subscript 0). The equations are expressed in terms of the total concentration of the chemical. The distribution between particulate and dissolved fractions is modeled using a linear partitioning model. The mass balance equations of the model can be expressed in a general form which is quite convenient for numerical solution. The layer 1 and 2 equations are:

$$\begin{aligned} H_1 \frac{dC_{T1}}{dt} &= K_{L01}\left(f_{d1}C_{T1} - C_{d0}\right) + w_{12}\,(f_{p2}C_{T2} - f_{p1}C_{T1}) \\ &\quad + K_{L12}\left(f_{d2}C_{T2} - f_{d1}\,C_{T1}\right) - k_1 H_1 C_{T1} + J_{T1} \end{aligned} \tag{2-5}$$

$$\begin{aligned} H_2 \frac{dC_{T2}}{dt} &= -\,w_{12}\,(f_{p2}C_{T2} - f_{p1}C_{T1}) - K_{L12}\left(f_{d2}C_{T2} - f_{d1}C\right) \\ &\quad - k_2\,H_2\,C_{T2} - w_2 C_{T2} + J_{T2} \end{aligned} \tag{2-6}$$

where:

C_{T1} = total concentration in layer 1 [M/L^3],
C_{T2} = total concentration in layer 2 [M/L^3],
f_{d1} = dissolved fraction in layer 1, $\dfrac{1}{1+m_2\pi_2}$
f_{p1} = 1 - f_{d1} = particulate fraction in layer 1,
f_{d2} = $\dfrac{1}{1+m_2\pi_2}$ dissolved fraction in layer 2,
C_{p2} = $f_{p2}\,C_{T2}$ = particulate concentration in layer 2 [M/L^3],
C_{d0} = dissolved concentration,
J_{T1} = total source into layer 1 [M/L^2-T],
J_{T2} = total source into layer 2 [M/L^2-T],
H_1 = depth of layer 1 [L],
H_2 = depth of layer 2 [L],
K_{L01} = aqueous mass transfer coefficient between layer 1 and the overlying water [L/T],
K_{L12} = aqueous mass transfer coefficient between layer 1 and layer 2 [L/T],
w_{12} = particle mixing velocity between layer 1 and layer 2 [L/T],
w_2 = sedimentation velocity out of layer 2 [L/T],

k_1 = first order decay rate coefficient removal process in layer 1 $[T^{-1}]$,
k_2 = first order decay rate coefficient removal process in layer 2 $[T^{-1}]$.

The dissolved and particulate concentrations and fractions are:

$C_{d1} = f_{d1}C_{T1}$ = dissolved concentration in layer 1 $[M/L^3]$,

$$f_{d1} = \frac{1}{1 + m_1\pi_1}$$

C_{p1} = $f_{p1}\ C_{T1}$ = particulate concentrations in layer 1 $[M/L^3]$,

C_{d2} = $f_{d2}\ C_{T2}$ = dissolved fraction in layer 2 $[M/L^3]$,

f_{p2} = $1 - f_{d2}$ = particulate fraction in layer 2,

where:

m_1 = solids concentration in layer 1 (aerobic layer) $[M/L^3]$,
m_2 = solids concentration in layer 2 (anerobic layer) $[M/L^3]$,
π_1 = partition coefficient in layer 1 $[L^3/M]$,
π_2 = partition coefficient in layer 2 $[L^3/M]$.

2.3.1 Surface Mass Transfer Coefficient and Reaction Velocities

The surface mass transfer coefficient, K_{L01}, quantifies the mixing between layer 1 and the overlying water. The critical observation is that it can be related to the sediment oxygen demand, SOD. The SOD is the mass flux of dissolved oxygen into the sediment. Thus, it can be calculated from the mass transfer equation:

$$D_1 \frac{d[O_2]}{dz}\Big|_{z=0} \approx D_1 \frac{[O_2(0)] - [O_2(H_1)]}{H_1} = \frac{D_1}{H_1}[O_2(0)] \tag{2-7}$$

where a straight line approximation to the derivative is used. The second equality follows from $[O_2(H_1)] = 0$, since H_1 is the depth of zero oxygen concentration. Therefore, the surface mass transfer coefficient can be expressed as:

$$K_{L01} = \frac{D_1}{H_1} = \frac{SOD}{\left[O_2(0)\right]} = s \tag{2-8}$$

which is the ratio of SOD and overlying water oxygen concentration. For notational simplicity this ratio is termed s.

The reaction rate in the aerobic layer is formulated as a conventional first order reaction with reaction rate constant k_1. The term in the layer 1 equation is k_1H_1. The depth of the aerobic zone follows from the definition of the surface mass transfer coefficient: $s = D_1/H_1$. Hence $k_1H_1 = k\ _1D_1/s$. The reaction velocity, which has units [L/T], is defined as:

$$\kappa_1 = \sqrt{D_1 k_1} \tag{2-9}$$

The square root is used to conform to the parameter group that appears in the spatially continuous form of the model. With these definitions the reaction rate - aerobic layer depth product becomes:

$$K_1 H_1 = \frac{\kappa_1^2}{s} \tag{2-10}$$

For convenience of nomenclature only, the reaction velocity in layer 2 may be defined as:

$$\kappa_2 = K_2 H_2 \tag{2-11}$$

It has units of [L/T]. However, it is not equivalent to the aerobic layer reaction velocities which include diffusion coefficient as well as a reaction rate constant.

With these definitions the layer 1 and 2 equations become:

$$\begin{aligned} H_1 \frac{dC_{T1}}{dt} &= s\left(f_{d1}C_{T1} - C_{d0}\right) + w_{12}\left(f_{p2}C_{T2} - f_{p1}C_{T1}\right) \\ &\quad + K_{L12}\left(f_{d2}C_{T2} - f_{d1}C_{T1}\right) - \frac{\kappa_1^2}{s} C_{T1} + J_{T1} \end{aligned} \tag{2-12}$$

$$H_2 \frac{dC_{T2}}{dt} = w_{12}\left(f_{d2}C_{T2} - f_{p1}C_{T1}\right) - K_{L12}\left(f_{d2}C_{T2} - f_{d1}C_{T1}\right) - \kappa_2 C_{T2} - w_2 C_{T2} + J_{T2} \qquad (2\text{-}13)$$

2.3.2 Particulate Phase Mixing

The rate of mixing of sediment particles by macrobenthos (bioturbation) has been quantified by estimating an apparent particle diffusion coefficient. The variation has been found to be proportional to the biomass of the benthos (Matisoft, 1982). In addition, it has been found that the benthic biomass is correlated to the carbon input to the sediment (Maughan, 1986, Robbins et al., 1989). In order to make the model self consistent - that is to use only internally computed variables in the parameterization - it seems reasonable to assume that benthic biomass is proportional to the labile carbon in the sediment, which is calculated by the model as $G_{POC,1}$. The temperature dependency of particle mixing has been accounted for by using an Arrhenius formulation.

A series of experiments have examined the relationship between particle mixing due to benthic organisms and the overlying water oxygen concentration. There is a general dependency of mixing rate on DO, with the lower rates occurring at the lower DO concentration. This dependency is modeled using a Michaelis Menton expression. The particle mixing mass transfer coefficient that results is:

$$w_{12}^{*} = D_p \frac{\theta_{Dp}^{(T-20)}}{H_2} \frac{G_{POC,1}}{G_{POC,R}} \frac{[O_2(0)]}{K_{M,Dp} + [O_2(0)]} \qquad (2\text{-}14)$$

with units [L/T]. The superscript * is used to denote this formulation from the final expression for w_{12} that is developed below. The parameter values are:

D_p = Diffusion coefficient for particle (m^2/d),
θ_{Dp} = Temperature coefficient for D_p
$G_{POC,R}$ = Reference concentration for $G_{POC,1}$ (mg/m^3),
$K_{M,Dp}$ = Particle mixing half saturation constant for oxygen (mg/L).

2.3.3 Benthic Stress

In addition to the reduction in particle mixing velocity due to the instantaneous oxygen concentration, it has been found necessary to include a more lasting effect. In particular, if anoxia occurs the benthic fauna population is reduced or eliminated. This is modeled using a first order differential equation that accumulates stress, S, when overlying water dissolved oxygen is below the particle mixing half saturation constant for oxygen, $K_{M,Dp}$. Thus:

$$\frac{dS}{dt} = -\,k_s S + \frac{K_{M,Dp}}{K_{M,Dp} + [O_2\,(O)]} \tag{2-15}$$

where:

S = Accumulated benthic stress [T],

k_s = First order decay coefficient for accumulated stress [T^{-1}].

The behavior of this formulation can be understood by evaluating the limiting steady state stresses at the two oxygen extremes:

$$[O_2(0)] \to 0 \quad k_s S \to 1 \quad (1 - k_s S) \to 0$$

$$[O_2(0)] \to \infty \quad k_s S \to 0 \quad (1 - k_s S) \to 1$$

Note that as $[O_2(0)]$ approaches zero at the onset of anoxia, the term $(1 - k_s S)$ is the proper variable to quantify the degree of benthic stress. The expression is unitless and requires no additional parameter - for example a half saturation constant for benthic stress. The final formulation for the particle mixing velocity which includes the benthic stress is:

$$w_{12} = w_{12}^{*} \min\left\{(1 - k_s S)\right\} \tag{2-16}$$

where w_{12}^{*} is defined above. The stress is continued at its minimum value through the end of the year, in order to conform to the observation that once the benthos has been suppressed by low oxygen, it does not recover until the next year.

2.3.4 Dissolved Phase Mixing

Dissolved phase mixing between layers 1 and 2 is via passive molecular diffusion which is enhanced by the mixing activities of the benthic organisms (bio-irrigation). This is modeled by increasing the diffusion coefficient by a factor of 10 over the molecular diffusion coefficient.

$$K_{L12} = \frac{D_d \theta_{Dd}^{(T-20)}}{H_2} \tag{2-17}$$

D_d = Pore water diffusion coefficient (m^2/day),
θ_{Dd} = Temperature coefficient for D_d.

2.3.5 Solids Burial

The deposition of solids to the sediment causes an increase in the depth of the sediment relative to a fixed datum. If the sediment surface is regarded as the point of reference, then the increase in the depth of sediment is a loss of mass due to burial from the active sediment layer.

w_2 = Sedimentation velocity (m/d)

2.3.6 Active Layer Depth

The active layer depth is chosen to represent the depth of organism mixing. Particles buried below this depth can longer be recycled to the aerobic layer. They are permanently buried.

H_2 = Depth of the anaerobic layer (m)

Table 2-1. Sediment Model Coefficients

Description	Notation	Value	Units
Aerobic layer solids concentration	m_1	0.2-1.2	kg/L
Anaerobic layer solids concentration	m_2	0.2-1.2	kg/L
Particle mixing diffusion coefficient	D_p	0.00006	m^2/d
Sedimentation velocity	w_2	0.25-0.75	cm/yr
Pore water diffusion coefficient	D_d	0.0005-0.0050	m^2/d
Temperature coefficient	θ_{Dp}	1.08-1.10	
Temperature coefficient	θ_{Dd}	1.10-1.117	
Water-sediment diffusion coefficient	D_{d0}	0.001	m^2/d
Temperature coefficient	$\theta_{D_{d0}}$	1.08	
Reaction velocity for nitrification-saltwater	κ_{nh4}	0.1313	m/d
Reaction velocity for nitrification-freshwater	κ	0.20	m/d
Ammonia partition coefficient	π_{nh4}	1.0	L/kg
Temperature coefficient	θ_{nh4}	1.123	
Nitrification half saturation constant for ammonia	k_{mnh4}	728.	mg N/L
Temperature coefficient	θ_{kmnh4}	1.125	
Nitrification half saturation constant for oxygen	k_{mnh4o2}	0.37	mg O_2/L
Aerobic denitrification velocity-saltwater	κ_{1no3}	1.25	m/d
Aerobic denitrification velocity-freshwater	κ_{1no3}	0.20	m/d
Anaerobic layer reaction velocity	κ_{2no3}	0.25	m/d
Temperature coefficient	θ_{no3}	1.08	
Reaction velocity for dissolved sulfide oxidation in the aerobic layer	κ_{d1}	0.2	m/d
Reaction velocity for particulate sulfide oxidation in the aerobic layer	κ_{p1}	0.4	m/d
Partition coefficient for sulfide in the aerobic layer	π_{1s}	100.	L/kg
Partition coefficient for sulfide in the anaerobic layer	π_{2s}	100.	L/kg
Temperature coefficient	θ_{dp1}	1.08	
Sulfide oxidation normalization constant for oxygen	k_{mhso2}	4.	mg O_2/L
First order reaction rate	k_{si}	0.5-0.75	/day
Silica saturation concentration	c_{sisat}	40000.	µg Si/L
Incremental partition coefficient for silica in the aerobic layer	$\Delta\pi_{1si}$	10.	
Partition coefficient for silica in the anaerobic layer	π_{2si}	100.	L/kg
Depth of sediment layer	h_{20}	0.1	m
Temperature coefficient	θ_{si}	1.10	

Table 2-1. Sediment Model Coefficients (Continued)

Description	Notation	Value	Units
Particulate biogenic silica half saturation constant for dissolution	k_{mpsi}	5.0E+07	mg Si/m^3
Overlying water oxygen concentration at which aerobic layer incremental partitioning starts to decrease	$O_{2critsi}$	2.0	mg O_2/L
Partition coefficient for phosphate in the anaerobic layer	$\pi_1 PO_{4n}$	20-1000	L/kg
Enhanced aerobic layer partition coefficient under fully oxic conditions	$\pi_1 PO_{4m}$	20-300	L/kg
Overlying water oxygen concentration at which aerobic layer incremental partitioning starts to decrease	O_{2crit}	2	mg O_2/L
Particle mixing half saturation constant for oxygen	k_{mo2Dp}	4.0	mg O_2/L
Temperature which benthic community begins to recover after an anoxic event	tempbnth	10.0	˚C
Rate at which benthic stress is dissipated	$k_{bnthstr}$	0.03	/d
Scale factor for enhancement of dissolved phase mixing due to benthic activity	k_{lbnth}	0.0	
Minimum particle mixing coefficient	D_{pmin}	3.0E-06	m2/d
Reaction velocity for methane oxidation in the aerobic layer	κ_{ch4}	0.2	m/d
Temperature coefficient	θ_{ch4}	1.08	
Reaction Rate Constant for Diagenesis -G1	$k_{GPOM,1}$	0.035	/day
Reaction Rate Constant for Diagenesis -G2	$k_{GPOM,2}$	0.0018	/day
Reaction Rate Constant for Diagenesis -G3	$k_{GPOM,3}$	0.0-1.0E-6	/day
Temperature Coefficient for Diagenesis - G1	θ_{G1}	1.10	
Temperature Coefficient for Diagenesis - G2	θ_{G2}	1.15	
Temperature Coefficient for Diagenesis - G3	θ_{G3}	1.17	

Table 2-1. Sediment Model Coefficients
(Continued)

Source	Distribution of Water Water Column POM Fractions To Each Class G1	G2	G3
Algal Carbon	0.6	0.2	0.2
Labile Particulate Organic Carbon	1.0	0.0	0.0
Refractory Particulate Organic Carbon	0.0	0.5	0.5
Algal Nitrogen	0.6	0.2	0.2
Labile Particulate Organic Nitrogen	1.0	0.0	0.0
Refractory Particulate Organic Nitrogen	0.0	0.6	0.4
AlgalPhosphorus	0.6	0.2	0.2
Labile Particulate Organic Phosphorus	1.0	0.0	0.0
Refractory Particulate Organic Phosphorus	0.0	0.5	0.5

GROUP P: SEDIMENT MODEL INPUT

P1. Print Options

```
          80
     Comment
 FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
       10          20           30             40
ISEDPRNT  IPRNTSED  TWARPSED     IGDSEDOPT
FORMAT ()
```

ISEDPRNT = sediment print control
= 0, do not print sediment input
= 1, print sediment input
IPRNTSED = print interval to save sediment computations (nominal = seconds)
TWARPSED = time-warp or units used for IPRNTSED. Normally IPRNTSED is input in units of seconds. The user may, however, use different units.
= SECS or secs
= MINS or mins
= HRS or hrs
= DAYS or days
IGDSEDOPT = global dump averaging option
= 0, no averaging
= 1, perform averaging

P2. Sediment Depths

```
          80
     Comment
 FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
     10               80
HSED(1,1)   ... HSED(NX,1)
   .
   .
   .
     10                   80
HSED(1,NY)   ... HSED(NX,NY)
FORMAT (8F10.3)
```

HSED(ISED) = sediment layer depth (cm)

P3. Sediment Initial Conditions

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALEIC
FORMAT (F10.2)

SCALEIC = scale factor for each sediment variable initial conditions

10 20 80
SCARAY(1,1) SCARAY(2,1) ... SCARAY(NX,1)
.
.
.
10 80
SCARAY(1,NY) ... SCARAY(NX,NY)
FORMAT (8E10.2)

SCARAY(IX,IY) = sediment initial condition for segment (IX,IY)

The comment line SCALEIC and SCARAY are repeated for each of the following variables used in the sediment nutrient flux model. The order of the initial conditions required for the sediment nutrient flux model is as follows:

CTEMP (IX,IY) = Initial sediment temperature (°C)
CPOP (IX,IY, 1) = G_1 Particulate Organic Phosphorus, POP ,(mg/m^3)
CPON (IX,IY, 1) = G_1 Particulate Organic Nitrogen, PON, (mg/m^3)
CPOC (IX,IY, 1) = G_1 Particulate Organic Carbon, POP, (mg/m^3)
CPOP (IX,IY, 2) = G_2 POP (mg/m^3)
CPON (IX,IY, 2) = G_3 PON, (mg/m^3)
CPOC (IX,IY, 2) = G_2 POC, (mg/m^3)
CPOP (IX,IY, 3) = G_3 POP, (mg/m^3)
CPON (IX,IY, 3) = G_3 PON, (mg/m^3)
CPOC (IX,IY, 3) = G_3 POC, (mg/m^3)
PO4T2 (IX,IY) = Layer 2 orthophosphate, PO_4, (mg/m^3)
NH4T2 (IX,IY) = Layer 2 ammonia, NH_4, (mg/m^3)
NO3T2 (IX,IY) = Layer 3 nitrate, NO_3, (mg/m^3)
H2ST2 (IX,IY) = Layer 2 hydrogen sulfide (in oxygen equivalents), H_2S, (mg O_2/m^3)
SIT2 (IX,IY) = Layer 2 silica, (mg/m^3)
BNTHSTRS (IX,IY) = Benthic stress
PO4T1 (IX,IY) = Layer 1 orthophosphate, PO_4, (mg/m^3)
NH4T1 (IX,IY) = Layer 1 ammonia, NH_4, (mg/m^3)

NO3T1 (IX,IY) = Layer 1 nitrate NO_3, (mg/m^3)

SIT1 (IX,IY) = Layer 1 silica, (mg/m^3)

H2ST1 (IX,IY) = Layer 1 hydrogen sulfide (in oxygen equivalents), H_2S, $(mg\ O_2/m^3)$

CH4T1 (IX,IY) = Layer 1 total methane (in oxygen equivalents), CH_4, (mgO_2/m^3)

CH4T2(IX,IY) = Layer 2 Total Methane (in oxygen equivalents), CH_4, (mgO_2/m^3)

SO4T2 (IX,IY) = Layer 2 total sulfate (in oxygen equivalents), SO_4, (mgO_2/m^3)

P4. Temperature Diffusion Coefficient, G Component Fractions and Diagenesis Rates

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
DIFFT
FORMAT (F10.0)

DIFFT = Water column-sediment layer temperature diffusion coefficient (cm^2/sec)

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SALTSW
FORMAT(F10.0)

SALTSW = salinity concentration for determining whether saltwater or freshwater nitrification and denitrification rates are applied. (If salinity is greater than SALTSW then saltwater values are applied.

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRPPH1(1)	FRPPH1(2)	FRPPH1(3)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRPPH2(1)	FRPPH2(2)	FRPPH2(3)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRPPH3(1)	FRPPH3(2)	FRPPH3(3)

FORMAT(3F10.0)

FRPPHI(I) = fractions of algal phosphorus going to G_1, G_2, G_3 sediment organic phosphorus for algal group I.

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRPOP(1)	FRPOP(2)	FRPOP(3)

FORMAT(3F10.0)

FRPOP(I) = fraction of non-algal/detrital POP going to G_1, G_2, G_3 sediment organic phosphorus

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRNPH1(1)	FRNPH1(2)	FRNPH1(3)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRNPH2(1)	FRNPH2(2)	FRNPH2(3)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRNPH3(1)	FRNPH3(2)	FRNPH3(3)

FORMAT(3F10.0)

FRNPHI(I) = fraction of algal nitrogen going to G_1, G_2, and G_3 sediment organic nitrogen for algal group I

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRPON(1)	FRPON(2)	FRPON(3)

FORMAT(3F10.0)

FRPON(I) = fraction of non-algal/detrital PON going to G_1, G_2, and G_3 sediment organic nitrogen

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRCPH1(1)	FRCPH1(2)	FRCPH1(3)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRCPH2(1)	FRCPH2(2)	FRCPH2(3)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRCPH3(1)	FRCPH3(2)	FRCPH3(3)

FORMAT(3F10.0)

FRCPHI(I) = fraction of algal carbon going to G_1, G_2, and G_3 sediment organic carbon from algal group I

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
FRPOC(1)	FRPOC(2)	FRPOC(3)

FORMAT(3F10.0)

FRPOC(I) = fraction of non-algal/detrital POC going to G_1, G_2, and G_3 sediment organic carbon

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60
KPDIAG(1)	DPTHTA(1)	KPDIAG(2)	DPTHTA(2)	KPDIAG(3)	DPTHTA(3)

FORMAT(6F10.0)

KPDIAG(I) = diagenesis reaction rates for POP G_1, G_2 and G_3, respectively, (1/day)
DPTHTA(I) = temperature coefficients for POP G_1, G_2 and G_3, respectively

10	20	30	40	50	60
KNDIAG(1)	DNTHTA(1)	KNDIAG(2)	DNTHTA(2)	KNDIAG(3)	DNTHTA(3)

FORMAT(6F10.0)

KNDIAG(I) = diagenesis reaction rates for PON G_1, G_2 and G_3, respectively, (1/day)
DNTHTA(I) = temperature coefficients for PON G_1, G_2 and G_3, respectively

10	20	30	40	50	60
KCDIAG(1)	DCTHTA(1)	KCDIAG(2)	DCTHTA(2)	KCDIAG(3)	DCTHTA(3)

FORMAT(6F10.0)

KCDIAG(I) = diagenesis reaction rates for POC G_1, G_2 and G_3, respectively, (1/day)
DCTHTA(I) = temperature coefficients for POC G_1, G_2 and G_3, respectively

10	20
KSI	THTASI

FORMAT(2F10.0)

KSI = Diagenesis reaction rate for Si, (1/day)
THTASI = Temperature coefficient for Si

P5. Sedimentation and Particle Mixing Rates

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

```
              10                  20                         80
VECTOR(1,1)     VECTOR(2,1)     ...   VECTOR(NX,1)
          .
          .
          .
              10                         80
VECTOR(1,NY)     ...    VECTOR(NX,NY)
FORMAT(8E10.2)
```

Comment and VECTOR(IX,IY) are repeated for the following variables:

VSED(IX,IY) = sedimentation velocity, (cm/yr)
VPMIX(IX,IY) = solid-phase mixing rate, (m^2/day) - D_p
VDMIX(IX,IY) = dissolved-phase mixing rate, (m^2/day) - D_d

P6. Sediment Model Constants

```
                  80
             Comment
 FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
          10             20                30
M1M2OPT   PIESIOPT   PIEPO4OPT
FORMAT(3F10.0)
```

M1M2OPT = M1,M2 input option
= 0, M1 and M2 are spatially constant
= 1, M1 and M2 are spatially variable
PIESIOPT = PIESI input option
= 0, Si partition coefficients are spatially constant
= 1, Si partition coefficients are spatially variable
PIEPO4OPT = PIEPO4 input option
= 0, PO_4 partition coefficients are spatially constant
= 1, PO_4 partition coefficients are spatially variable

If MIM20PT = 0 (spatially constant M1 and M2)

```
                  80
             Comment
 FORMAT (A80)
```

Comment = Comment line (ignored by RCA)

```
 10    20           30           40
M1    M2    THTADp    THTADd
FORMAT(4F10.0)
```

M1 = aerobic layer solids concentration, (kg/l)
M2 = anaerobic layer solids concentration, (kg/l)
THTADp = temperature coefficient for D_p
THTADd = temperature coefficient for D_d

If MIM20PT = 1 (spatially variable M1 and M2)

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALE
FORMAT (F10.0)

SCALE = scale factor

10 20 80
M1(1,1) M1(2,1) . . . M1(NX,1)
.
.
.
M1(1,NY) M1(2,NY) . . . M1(NX,NY)
FORMAT(8F10.0)

M1(IX,IY) = aerobic layer solids concentration for sediment segment IX,IY (kg/L)

10
SCALE
FORMAT (F10.0)

SCALE = scale factor

80
M2(1,1) M2(2,1) . . . M2(NX,1)
.
.
.
M2(1,NY) M2(2,NY) . . . M2(NX,NY)
FORMAT(8F10.0)

M2(IX,IY) = an aerobic layer solids concentration for sediment segment IX,IY (kg/L)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20
THTADp	THTADd

FORMAT (2F10.0)

THTADp = temperature coefficient for D_p
THTADd = temperature coefficient for D_d

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20
Dd0	THTADd0

FORMAT(2F10.0)

Dd0 = minimum pore water diffusion coefficient (m^2/day)
THTADd0 = temperature coefficient for Dd0

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60
KAPPNH4S	PIENH4	THTANH4S	KMNH4	THTAKMNH4	KMNH4O2

FORMAT(6F10.0)

KAPPNH4S = nitrification velocity in saltwater, (m/d)
PIENH4 = partition coefficient for nitrogen, (L/kg)
THTANH4S = nitrification temperature coefficient in saltwater
KMN4 = ammonia half saturation constant, (mg N/L)
THTAKMN4 = temperature coefficient
KMNH402 = oxygen half saturation constant, (mg O_2/L)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20
KAPPNH4F	THTANH4F

FORMAT(2F10.0)

KAPPNH4F = nitrification velocity in freshwater, (m/d)
THTANH4F = nitrification temperature coefficient in freshwater

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
KAPP1NO3S	K2NO3S	THTANO3S

FORMAT(3F10.0)

KAPP1NO3S = aerobic denitrification velocity in seawater, (m/d)
K2NO3S = anaerobic layer denitrification rate for seawater, (1/d)
THTANO3S = diagenesis temperature coefficient in seawater

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30
KAPP1NO3F	K2NO3F	THTANO3F

FORMAT(3F10.0)

KAPP1NO3F = aerobic denitrification velocity in freshwater, (m/d)
K2NO3F = anaerobic layer denitrification rate for freshwater, (1/d)
THTANO3F = diagenesis temperature coefficient in freshwater

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60
KAPPD1	KAPPP1	PIE1S	PIE2S	THTAPD1	KMHSO2

FORMAT(6F10.0)

KAPPD1 = reaction velocity for dissolved sulfide oxidation in the aerobic layer, (m/day)
KAPPP1 = reaction velocity for particulate sulfide oxidation in the aerobic layer, (m/day)
PIE1S = partition coefficient for sulfide in the aerobic layer, (L/kg)
PIE2S = partition coefficient for sulfide in the aerobic layer, (L/kg)
THTAPD1 = temperature coefficient for sulfide oxidation

KMHSO2 = sulfide oxidation normalization constant for oxygen, (mgO_2/L)

If PIESIOPT =0 (PIE1SI and PIE2SI are spatially constant)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60	70	80
CSISAT	PIE1SI	PIE2SI	KSI	THTASI	KMPSI	OCRITSI	JSIDETR

FORMAT(8F10.0)

CSISAT = silica saturation concentration, (mg Si/L)
PIEISI = partition coefficient for silica in aerobic layers, (L/kg)
PIE2SI = partition coefficient for silica in anaerobic layer, (L/kg)
KSI = first order reaction rate, (1/day)
THTASI = temperature coefficient
KMPSI = half saturation constant, (mg Si/g)
O2CRITSI = overlying water oxygen concentration at which aerobic layer incremental, partitioning starts to decrease (mg O_2/L)
JSIDETR = flux of detrital silica, (mg Si/m^2 - d)

If PIESIOPT =1 (PIE1SI and PIE2SI are spatially variable)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALE

FORMAT (F10.0)

SCALE = scale factor

10	20	80
PIE1SI(1,1)	PIE1SI(2,1) . . .	PIE1SI(NX,1)

.
.
.

10	80
PIE1SI(1,NY) . . .	PIE1SI(NX,NY)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALE

FORMAT (F10.0)

SCALE = scale factor

10	20	80
PIE2SI(1,1)	PIE2SI(2,1) . . .	PIE2SI(NX,1)

.
.
.

10	80
PIE2SI(1,NY) . . .	PIE2SI(NX,NY)

PIE1SI(IX,IY) = aerobic layer Si partition coefficient (L/kg)
PIE2SI(IX,IY) = anaerobic layer Si partition coefficient (L/kg)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60
CSISAT	KSI	THTASI	KMPSI	O2CRITSI	JSIDETR

CSISAT = silica saturation concentration, (mg Si/L)
KSI = first order reaction rate, (1/day)
THTASI = temperature coefficient
KMPSI = half saturation constant, (mg Si/g)
O2CRITSI = overlying water oxygen concentration at which aerobic layer incremental, partitioning starts to decrease (mg O_2/L)
JSIDETR = flux of detrital silica, (mg Si/m^2 - d)

If PIEPO4OPT =0 (PIE1PO4M and PIE1PO4N are spatially constant)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40
PIE1PO4M	PIE1PO4N	O2CRIT	KMO2DP

FORMAT(4F10.0)

PIE1PO4M = incremental partition coefficient for phosphate in aerobic layer, (L/kg)
PIE1PO4N = partition coefficient for phosphate in the anaerobic layer, (L/kg)
O2CRIT = overlying water oxygen concentration at which aerobic layer incremental partitioning starts to decrease, (mg O_2/L)
KMO2DP = half saturation constant, (mg Si/g)

If PIEPO4OPT = 1 (PIE1PO4 and PIE2PO4 are spatially variable)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALE

FORMAT (F10.0)

SCALE = scale factor

10 20 80
PIE1PO4(1,1) PIE1PO4(2,1) . . . PIE1PO4(NX,1)
.
.
.
10 80
PIE1PO4(1,NY) . . . PIE1PO4(NX,NY)

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
SCALE
FORMAT (F10.0)

SCALE = scale factor

10 20 80
PIE2PO4(1,1) PIE2PO4(2,1) . . . PIE2PO4(NX,1)
.
.
.
10 80
PIE2PO4(1,NY) . . . PIE2PO4(NX,NY)

PIE1PO4(IX,IY) = aerobic layer PO4 partition coefficient (L/kg)
PIE2PO4(IX,IY) = anaerobic layer PO4 partition coefficient (L/kg)

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 20
02CRIT KMO2DP

O2CRIT = overlying water oxygen concentration at which aerobic layer incremental partitioning starts to decrease (mg O_2/L)

KMO2Dp = half saturation constant for particle mixing (mgO_2/L)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40
TEMPBNTH	KBNTHSTR	KLBNTH	DPMIN

FORMAT(4F10.0)

TEMPBNTH = benthic temperature switch (°C)
KBNTHSTR = benthic stress decay rate constant (1/day)
KLBNTH = benthic stress enhancement constant
DPMIN = minimum value for physical benthic mixing, (m^2/day)

80
Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10	20	30	40	50
KAPPCH4	THTACH4	KMCH402	KMSO4	SO4OMG

FORMAT(5F10.0)

KAPPCH4 = reaction velocity for methane production (??/day)
THTACH4 = temperature coefficient for methane production
KMCH4O2 = half saturation coefficient for methane production (mg O2/L)
KMS04 = half saturation coefficient for sulfate (mg/L)
SO4OMG = overlying water sulfate concentration (mg s/L)

Table 2-2 presents a sample input deck for the sediment model coefficient set.

TABLE 2-2. SAMPLE INPUT DECK FOR THE SEDIMENT MODEL COEFFICIENT SET

```
C ISEDPRNT  IPRNTSED  TWARPSED IGDSEDOPT
         0     864000     SECS         1
C  Sediment depths (cm)
       0.       0.00       0.0       0.0
       0.      10.00      10.0       0.0
       0.      10.00      10.0       0.0
       0.       0.00       0.0       0.0
C  scale factor / temperature initial conditions (Deg C)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0       3.2       3.2       0.0
       0.0       3.2       3.2       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G1 POP initial conditions (mg P/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0     1320.     1320.       0.0
       0.0     1320.     1320.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G1 PON initial conditions (mg N/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0    12400.    12400.       0.0
       0.0    12400.    12400.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G1 POC initial conditions (mg C/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0    61400.    61400.       0.0
       0.0    61400.    61400.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G2 POP initial conditions (mg P/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0     8680.     8680.       0.0
       0.0     8680.     8680.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G2 PON initial conditions (mg N/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0    92700.    92700.       0.0
       0.0    92700.    92700.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G2 POC initial conditions (mg C/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0   410000.   410000.       0.0
       0.0   410000.   410000.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G3 POP initial conditions (mg P/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0    58100.    58100.       0.0
       0.0    58100.    58100.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G3 PON initial conditions (mg N/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0   480000.   480000.       0.0
       0.0   480000.   480000.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / G3 POC initial conditions (mg C/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0  4210000.  4210000.       0.0
       0.0  4210000.  4210000.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / Biogenic Si initial conditions (mg Si/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0  5470000.  5470000.       0.0
       0.0  5470000.  5470000.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / Layer 2 Total Inorganic PO4 (mg P/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0    11500.    11500.       0.0
       0.0    11500.    11500.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / Layer 2 Total NH4 (mg N/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0     8770.     8770.       0.0
```

TABLE 2-2. SAMPLE INPUT DECK FOR THE SEDIMENT MODEL COEFFICIENT SET (Cont.).

```
      0.0     8770.     8770.      0.0
       0.0       0.0       0.0       0.0
C  scale factor / Layer 2 Nitrate (mg N/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0      250.      250.       0.0


       0.0      250.      250.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / Layer 2 Total Sulfide (as O2 equivalents) (mg O2/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0     1180.     1180.       0.0
       0.0     1180.     1180.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / Layer 2 Total Inorganic Si (mg Si/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0    22700.    22700.       0.0
       0.0    22700.    22700.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / Benthic Stress initial conditions
 0.100E+01
       0.       0.00       0.0       0.0
       0.      11.00      11.0       0.0
       0.      11.00      11.0       0.0
       0.       0.00       0.0       0.0
C  scale factor / Layer 1 Total Inorganic PO4 (mg P/m**3)
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0    16000.    16000.       0.0
       0.0    16000.    16000.       0.0
       0.0       0.0       0.0       0.0
C  scale factor / Layer 1 Total Inorganic NH4 (mg N/m**3)
 0.100E+01
       0.        0.0       0.0       0.0
       0.       35.0       35.       0.0
       0.       35.0       35.       0.0
       0.        0.0       0.0       0.0
C  scale factor / Layer 1 NO3 (mg N/m**3)
 0.100E+01
       0.        0.0       0.0       0.0
       0.       343.      343.       0.0
       0.       343.      343.       0.0
       0.        0.0       0.0       0.0
C  scale factor / Layer 1 Total Inorganic Si (mg Si/m**3)
 0.100E+01
       0.        0.0       0.0       0.0
       0.      8000.     8000.       0.0
       0.      8000.     8000.       0.0
       0.        0.0       0.0       0.0
C  scale factor / Layer 1 Sulfide (in oxygen equivalents) (mg O2/m**3)
 0.100E+01
       0.        0.0       0.0       0.0
       0.       0.02      0.02       0.0
       0.       0.02      0.02       0.0
       0.        0.0       0.0       0.0
C  scale factor / Layer 1 Methane (in oxygen equivalents) (mg O2/m**3)
 0.100E+01
       0.        0.0       0.0       0.0
       0.       0.02      0.02       0.0
       0.       0.02      0.02       0.0
       0.        0.0       0.0       0.0
C  scale factor / Layer 2 Methane (in oxygen equivalents) (mg O2/m**3)
 0.100E+01
       0.        0.0       0.0       0.0
       0.        5.0       5.0       0.0
       0.        5.0       5.0       0.0
       0.        0.0       0.0       0.0
C  scale factor / Layer 2 Sulfate (in oxygen equivalents) (mg O2/m**3)
 0.100E+01
       0.        0.0       0.0       0.0
       0.        0.9       0.9       0.0
       0.        0.9       0.9       0.0
       0.        0.0       0.0       0.0
C    Difft
   0.00180
C   SALTSW
      0.00                             SALTSW
C FRPPH1-G1 FRPPH1-G2 FRPPH1-G3    fractions to G1, G2, G3 P for Algal Group 1
     0.650     0.200     0.150     FRPPH1 (G1,G2,G3)
C FRPPH2-G1 FRPPH2-G2 FRPPH2-G3    fractions to G1, G2, G3 P for Algal Group 2
```

TABLE 2-2. SAMPLE INPUT DECK FOR THE SEDIMENT MODEL COEFFICIENT SET (Cont.).

```
     0.650     0.200     0.150     FRPPH2 (G1,G2,G3)
C FRPPH3-G1 FRPPH3-G2 FRPPH3-G3    fractions to G1, G2, G3 P for Algal Group 3
     0.650     0.200     0.150     FRPPH2 (G1,G2,G3)
C FRPOP-G1  FRPOP-G2  FRPOP-G3    fractions to G1, G2, G3 P for detrital POP
     0.650     0.200     0.150     FRPOP (G1,G2,G3)
C FRNPH1-G1 FRNPH1-G2 FRNPH1-G3    fractions to G1, G2, G3 N for Algal Group 1
     0.650     0.250     0.100     FRNPH1 (G1,G2,G3)
C FRNPH2-G1 FRNPH2-G2 FRNPH2-G3    fractions to G1, G2, G3 N for Algal Group 2
     0.650     0.250     0.100     FRNPH2 (G1,G2,G3)
C FRNPH3-G1 FRNPH3-G2 FRNPH3-G3    fractions to G1, G2, G3 N for Algal Group 3
     0.650     0.250     0.100     FRNPH2 (G1,G2,G3)
C FRPON-G1  FRPON-G2  FRPON-G3    fractions to G1, G2, G3 N for detrital PON
     0.650     0.250     0.100     FRPON (G1,G2,G3)
C FRCPH1-G1 FRCPH1-G2 FRCPH1-G3    fractions to G1, G2, G3 C for Algal Group 1
     0.650     0.200     0.150     FRCPH1 (G1,G2,G3)
C FRCPH2-G1 FRCPH2-G2 FRCPH2-G3    fractions to G1, G2, G3 C for Algal Group 2
     0.650     0.200     0.150     FRCPH2 (G1,G2,G3)
C FRCPH3-G1 FRCPH3-G2 FRCPH3-G3    fractions to G1, G2, G3 C for Algal Group 3
     0.650     0.200     0.150     FRCPH2 (G1,G2,G3)
C FRPOC-G1  FRPOC-G2  FRPOC-G3    fractions to G1, G2, G3 C for detrital POC
     0.650     0.200     0.150     FRPOC (G1,G2,G3)
C KPDIAGG1   THETAG1  KPDIAGG2   THETAG2  KPDIAGG3   THETAG3    POP Diag Rates
 0.0350000     1.100 0.0018000     1.150 0.0000010     1.170
C KNDIAGG1   THETAG1  KNDIAGG2   THETAG2  KNDIAGG3   THETAG3    PON Diag Rates
 0.0350000     1.100 0.0018000     1.150 0.0000010     1.170
C KCDIAGG1   THETAG1  KCDIAGG2   THETAG2  KCDIAGG3   THETAG3    POC Diag Rates
 0.0350000     1.100 0.0018000     1.150 0.0000010     1.170
C  KSiDiag     THETA                                        Biogenic Diag Rate
     0.500     1.100
C   Sedimentation or Burial Rates  (cm/yr)
C Scale Factor
 0.100E+01
       0.       0.00       0.0       0.0
       0.      0.250      0.25       0.0
       0.      0.250      0.25       0.0
       0.       0.00       0.0       0.0
C   Particle or solid phase mixing rate (m2/day)
C Scale Factor
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0 0.120E-03 0.120E-03       0.0
       0.0 0.120E-03 0.120E-03       0.0
       0.0       0.0       0.0       0.0
C   Dissolved phase mixing rate (m2/day)
C Scale Factor
 0.100E+01
       0.0       0.0       0.0       0.0
       0.0 0.100E-02 0.100E-02       0.0
       0.0 0.100E-02 0.100E-02       0.0
       0.0        0.0       0.0       0.0
C  M1M2OPT  PIESIOPT PIEPO4OPT   (0=spatially constant,1=variable)
         0         0         0
C       M1        M2   ThetaDp   ThetaDd
     0.500     0.500    1.1500    1.1500
C      Ddo  ThetaDdo
    0.0010    1.0800
C KappNH4S    PIENH4 ThetaNH4S     KMNH4 ThtaKmNH4   KMNH4O2    (saltwater values)
    0.1313    1.0000    1.0800  728.0000    1.1250    0.7400
C KappNH4F ThetaNH4F    (freshwater values)
    0.2000    1.0800
C KappNO3S    K2NO3S ThetaNO3S    (saltwater values)
    0.0500    0.1000    1.3000
C KappNO3F    K2NO3F ThetaNO3F    (freshwater values)
    0.1000    0.2500    1.0800
C    Kappd1    Kappp1     PIE1S     PIE2S  ThetaPD1    KMHSO2
    0.2000    0.4000  100.0000  100.0000    1.0800    4.0000
C    CSiSat    PIE1Si    PIE2Si       KSi  ThetaSi      KMPSi  O2CritSi    JsiDetr
40000.0000    15.000    100.00    0.5000    1.1000   5.0E+07    2.0000       060.
C  PIEPO4M  PIE1PO4N    O2Crit    KMO2Dp
      20.0      20.0      2.00      4.00
C TempBnth  KBnthStr    K1Bnth     Dpmin
   10.0000    0.0300    0.0000    0.0000
C  KappCh4  ThetaCh4   KMCH4O2     KMSO4
      0.20      1.08      0.20      0.10
```

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APPENDIX B

PATHOGEN MODEL

PATHOGEN MODEL

Despite significant efforts and expenditures by federal, state, and local government to reduce the sources of pathogenic bacteria, associated with human health risks and diseases, to receiving waters, pathogens continue to be an issue when trying to meet the "swimmable" goals of the Clean Water Act. This is particularly the case for waters that receive combined sewer overflows (CSOs) from the nation's larger and older cities, wherein both sanitary and stormwater are conveyed in the same sewer system. However, modeling of the major waterborne pathogens of concern (including *V. Cholerae, Salmonellae, and Shigella* species) is usually not practiced due to the difficulty in measuring these organisms directly in the receiving waters. Rather surrogate indicator organisms, such as total and fecal coliform are modeled. More recently, through the Coastal Health Act of 2000, the USEPA is requiring that the coastal states implement the enterococci criteria for marine waters originally developed in the 1986 "Ambient Water Quality Criteria for Bacteria - 1986" guidance document. Therefore, the pathogen model developed by HydroQual includes state-variables for total and fecal coliform and enterococcus.

The mathematical framework employed in the pathogen model is the same mass-balance approach detailed in Appendix A - Integrated Eutrophication and Sediment Nutrient Flux Model, only the state-variables and reaction rates differ. The pathogen model includes the following state-variables:

1. Salinity (ppt)
2. Tracer (mg/L)
3. Total Coliform Bacteria (#/100 mL)
4. Fecal Coliform Bacteria (#/100 mL)
5. Enterococci (#/100 mL)

Note: when inputting loads of coliform bacteria or enterococci, the user should use the following procedure:

bacterial load = wastewater (or CSO) flow * coliform concentration * conversion factor

where the coliform concentration is in units of #/100 mL and the conversion factor is:

Units of wastewater flow	Conversion factor
m^3/day	0.001
m^3/sec	86.4
MGD	3.785
cfs	2.446

At the present time, the HydroQual pathogen model only incorporates a first-order decay or die-off rate for coliform bacteria and enterococcus. The model does not account for any post-discharge growth of the organisms in the receiving water. The tracer variable is included in the model framework should the user wish to "tag" or follow the spatial distribution of a particular WWTP(s), CSO(s), or separate sewer overflow (SSOs). The present framework permits the coliform/enterococcus die-off rate to be a function of temperature, sunlight, and, for estuarine/coastal systems, salinity. The following equation represents the die-off rate for total and fecal coliform and entrerococcus:

$$k_{die-off} = (k_{base} + k_{sal}(S)) \cdot \theta_{sal}^{(T-20)} + k_{light} \cdot f(I) \qquad (1)$$

where:

$k_{die\text{-}off}$ = composite die-off rate (/day),
k_{base} = base die-off rate (/day),
k_{sal} = salinity dependent die-off rate (/ppt-day),
S = concentration of salinity (ppt),
θ = temperature correction coefficient for die-off rate,
T = temperature (deg C),
k_{light} = light-dependent die-off rate (ly-day),
$f(I)$ = depth- and time-integrated light intensity (ly).

The function, f(I), may be evaluated as follows:

$$f(I) = \frac{I_0(t)}{K_e H}(1 - \exp(-K_e H) \qquad (2)$$

where:

$I_0(t)$ = solar radiation at water surface (or at surface of model segment if water column is vertically segmented), (ly),
K_e = extinction coefficient (/m),
H = depth of water column (or depth of model segment if the water column is vertically segmented in the model) (m).

The following presents the structure of the parameters, constants, and time-variable functions input file for running the pathogen model.

2-D Parameters

Number	Name	Description
1	KEBS	= extinction coefficients (used when KEOPT = 1 or 3) (/m),

Constants

Number	Name	Description
1	KCBC	= base die-off rate for coliform bacteria at 20 deg C (/day),
2	KCBT	= temperature correction coefficient,
3	KCSAL	= salinity-dependent coliform die-off rate (/ppt-day),
4	KCLGHT	= sunlight-dependent coliform die-off rate (/ly-day),
5	SOLAR	= option to include sunlight-dependent die-off rate, = 0, do not include sunlight effects on die-off rate, = 1, include sunlight effects on die-off rate,
6	KEBC	= base die-off rate for enterococcus at 20 deg C (/day),
7	KEBT	= temperature correction coefficient,
8	KESAL	= salinity-dependent enterococcus die-off rate (/ppt-day),

9 KELGHT = sunlight-dependent coliform die-off rate (/ly-day),

10 KEOPT = method for inputting extinction coefficients,
- = 0, K_e is a constant (i.e., spatially and temporally invariant),
- = 1, K_e is spatially variable, but constant in time (uses the 2-D parameter, KEBS)
- = 2, K_e is time-variable (uses the time-variable function KETVF), but spatially invariant,
- = 3, K_e is spatially variable and can vary in time, using the 2-D parameter, KEBS, and the time-variable function, KETVF,
- = 4, K_e is fully variable in time and space, with input coming from a separate input file (kebs.inp),

11 KECONST = base extinction coefficient (used when KEOPT = 0 or 2) (/m),

Time-Variable Functions

Number	Name	Description
1	ITOTSF	= total daily solar radiation (used when KEOPT = 2,3 or 4) (/m),
2	F	= fraction of daylight (used when KEOPT = 2, 3, or 4),
3	KETVF	= time-variable scaling factor for extinction coefficients (used when KEOPT = 2 or 3).

APPENDIX C

RESIDENCE TIME/TRACER MODEL

RESIDENCE TIME/DYE-TRACER SUBROUTINE

One method for determining whether the transport fields computed by the hydrodynamic model, which are to be used to advect and disperse water quality variables of interest within RCA, are correct is to compare them to observed data. For estuarine systems, these comparisons are usually made using observed water elevations, current meter data, and salinity, temperature, and density data. However, in addition, in special cases tracers, such as Rhodamine dye or SF_6 (sulfur hexafluoride, are used to provide data sets for calibration of hydrodynamic models, particularly when applied to freshwater systems.

In addition, it is often useful to know the residence time of a region or portion of a waterbody. This information can be used to estimate how quickly a contaminant is flushed from that region or portion of the study domain. One way of determining the residence time of the region of interest is to perform model simulations using "conservative tracers or dyes."

Therefore, a TUNER subroutine has been developed that can be used to simulate the transport of a tracer within a study domain and that can be used to estimate the residence time of the tracer within a portion of the model domain or within the entire model domain. The mathematical framework employed in the tracer model is the same mass-balance approach detailed in Appendix A - Integrated Eutrophication and Sediment Nutrient Flux Model, only the state-variables differ. The tracer model has only one state-variable - the tracer or dye (actually the code provided can be quickly expanded to include three tracers or dyes by "un-Commenting" some of the FORTRAN code):

1. Tracer (mg/L)

The residence time or dye model is set up so that, in addition to putting a tracer or dye within the entire model domain, one can initialize only a portion of the model domain with the tracer and then have the model determine (1) the mass of tracer remaining within the initialized portion of the model domain, (2) a user specified portion of the model domain, as well as, (3) the mass of tracer left within the entire model domain. One can then post-process the model outputs to estimate the residence time of the dye using the commonly accepted definition of one *e*-folding time (one *e*-folding is defined as exp(-1) or the time at which 0.3679 of the initial mass remains within the region or the study domain).

The following presents the structure of the parameters, constants, and time-variable functions input file for running the pathogen model.

3-D Parameters

Number	Name		Description
1	DYE1IC3	=	initial conditions for tracer or dye (mg/L),
2	DOMAIN1	=	region of interest for determining residence time

2-D Parameters

Number	Name		Description
1	DYE1IC2	=	initial conditions for tracer or dye (mg/L),
2	DOMAIN1	=	region of interest for determining residence time

Constants Number	Name	Description
1	DYEDIS1	= dye distribution option, = 0, assign initial tracer concentrations uniformly in the vertical plane of the model as determined by the 2-D parameter DYE1IC2 = 1, assign initial tracer concentrations on a model segment by model segment basis as determined by the 3-D parameter DYE1IC3 (permits one to look at residence time of surface layer versus bottom layer)
2	TIMEDYE1	= time to release the tracer or dye (days),
3	DECAY1	= decay rate of tracer or dye (1 day)

Time-Variable Functions

No time-variable functions are required.

APPENDIX D

DESCRIPTION OF RCA OUTPUT FILE FORMATS

FILE DESCRIPTIONS FOR RCAF OUTPUT FILES
VERSION 3.0 OF RCA

The water quality modeling program, RCA, creates a number of output files (known as RCAF files) containing various types of model computations that (1) can be visualized by the user via GDP or other post-processing software, (2) can be used to "cycle" model runs, and (3) can provide for mass balance and flux balance analyses of a system. Currently there are four types of files saved by RCA: (1) global dump or map files, (2) detailed dump or history files, (3) "end of simulation" concentration files, and (4) mass balance and flux balance files. The global or map file provide a snapshot of the entire model domain for the key water quality variables, while the detailed or history file provides more "detailed" information about the model simulation for a more limited number of model segments within the model domain. The "end of simulation" concentration files contain the concentrations for all model segments for all systems at the end of the simulation. These files can be used by the user to cycle or "hot-start" a subsequent simulation, if one desires the model to achieve a "new" dynamic equilibrium in response to reductions in pollutant inputs or a management scenario. The mass balance/flux balance files provide information that permits a user to develop a mass balance analysis for a system or to perform a flux balance analysis in a certain portion(s) of the model domain. In order to restrain the physical size of each of the RCAF files, and thus reduce required physical disc-size requirements, all RCAF files are written in binary (rather than ASCII format). The following provides a more detailed description of the content and 'format' of each of the RCAF output files.

Global Dump Files - RCAF10 and RCAF11

The RCAF10 file provides information concerning the size of the model, the number of systems, the number of global dumps saved, the variable names, and the times for which the global information was saved. The RCAF11 file contains the concentrations of the key water quality variables within the model domain.

RCAF10 (internal RCA file number 10)

Record 1: NX,NY,NZ,NOSYS,NGDMP

where:	NX	number of computational elements in the x-direction (Integer)
	NY	number of computational elements in the y-direction (Integer)
	NZ	number of vertical layers (Integer)
	NOSYS	number of state-variables in the model (Interger)
	NGDMP	number of global dumps saved by the kinetic subroutine in RCAF11 (Integer)

Record 2: SYNAME(NGDMP)

where:	SYNAME	a vector (NGDMP elements long) that contains the names of the water quality parameters saved in the RCAF11 file (Character*8)

Record 3: SYSGDP(40)

where:	SYSGDP	a vector (40 elements long) that contains the system bypass information for the model run (Integer*2). Used primarily by HydroQual's in-house post-processing software.

Record 4: FSM(NX,NY)
where: FSM an array (NX x NY) containing the land-mask information for the model grid (Real). The following convention is used: water=1, land=0, boundaries=-1 or -2.

Records 5 -> TIME
where: TIME times at which the global dumps were written to the disk. Number of records = (total length of the simulation time ÷ global dump interval) + 1 (for the initial conditions).

RCAF11 (internal RCA file number 11)

Records 1 -> CARAY
where CARAY arrays (each NX x NY x NZ) containing the concentrations for each model segment in the model domain for each water quality variable of interest (Real). Record 1 contains the CARAY for variable 1, record 2 for variable 2, ..., record NGDMP for variable NGDMP. Record NGDMP+1 starts with variable 1 again, but for the next time record.

Detailed Dump Files - RCAF12 and RCAF13

RCAF12 (internal RCA file number 12)

Record 1: NDMPS
where NDMPS number of segments selected for saving detailed dumps (Integer).

Record 2: ((IFDMPS(I,J),J=1,3),I=1,NDMPS)
where IFDMP(I,J) contains the x cell number (j=1), the y cell number (j=2), and the z or sigma-layer cell number (j=3) for each of the segments saved (Integer).

Record 3: DDGDPBY(40)
where: DDGDPBY a vector (40 elements long) that contains the system bypass information for the model run (Integer*2). Used primarily by HydroQual's in-house post-processing software.

Record 4: DDNAMES(NOSYS,5)
where: DDNAMES a vector (NOSYS x 5 elements long) that contains the names of the water quality parameters saved in the RCAF13 file (Character*8). Each model system or state-variables has provision for saving 5 pieces or information (state-variable concentrations, combinations of state-variables, reaction terms, etc.). The specific information saved for each system is determined in the user's kinetic subroutine TUNER.

Record 5 -> TIME
where: TIME times for which the detailed dumps were saved (Real).

RCAF13 (internal RCA file number 13)

Records 1 -> BUFFER(50000)

where: BUFFER an array (50000 elements long) containing the detailed dumps (Real). The information for each system is packed into the 'buffer' as follows (assume NOSYS=25):

BUFFER(1-5) = the five pieces of information for the first IFDMP for system 1
BUFFER(6-10) = the five pieces of information for the first IFDMP for system 2
.
.
.
BUFFER(121-125) = the five pieces of information for the first IFDMP for system 25
BUFFER(126-130) = the five pieces of information for the second IFDMP for system 1
BUFFER(131-135) = the five pieces of information for the second IFDMP for system 2
.
.
.
BUFFER(246-250) = the five pieces of information for the second IFDMP for system 25
BUFFER(251-255) = the five pieces of information for the third IFDMP for system 1
BUFFER(256-260) = the five pieces of information for the third IFDMP for system 2
etc.

Note: not all of the buffer will be used, only NDMPS*5*NOSYS elements contain actual model computations (the remaining values should be zero).

Sediment Dump File - RCAF14

The RCAF14 file contains information from the sediment flux model (SFM) if used. RCAF14 looks like a global dump or map file, since it contains information generated by the SFM for all active model segments in the model domain (note: only the water segments corresponding to FSM(I,J)=1).

RCAF14 (internal RCA file number 14)

Record 1: FSM(NX,NY)

where: FSM an array (NX x NY) containing the land-mask information for the model grid (Real). The following convention is used: water=1, land=0, boundaries=-1 or -2.

Records 2 -> TIME,(SED(I),I=1,76)

where: TIME times at which the SFM info was saved (REAL)

SED a vector (76 elements long) containing information generated by the sediment flux model (REAL). The SED information is written for each active (FSM=1) segment using the following DO-loop sequence:

```
DO ICOL=1,NY
  DO IROW=1,NX
        WRITE(14)   TIME,SED
  ENDDO
ENDDO
```

The following NAMES have been assigned to the SED vector:
SED(1-5): ctemp,pop1r,pop2r,pop3r,popr
SED(6-10): pon1r,pon2r,pon3r,ponr,poc1r
SED(11-15): poc2r,poc3r,pocr,po4t2r,hst2r
SED(16-20): sit2r,psiavr,jpop,jpon,jpoc
SED(21-25): o20,csod,sod,s,jdiagp
SED(26-30): jdiagn,jdiagc,jo2nh4,xjco2av,xjc1av
SED(31-35): jpo4,jnh4,jno3,jhs,jsi
SED(36-40): jch4aq,jch4g,h1,po40,po41
SED(41-45): po42,po4t2,nh40,nh41,nh42
SED(46-50): nh4t2,no30,no31,no32,no3t2
SED(51-55): hs1,hs2,hst2,si0,si1
SED(56-60): si2,sit2,bnthden,ch41,ch42
SED(61-65): ch4t2,so41,so42,so4t2,flxpopG1
SED(66-70): flxpopG2,flxpopG3,flxponG1,flxponG2,flxponG3
SED(71-75): flxpocG1,flxpocG2,flxpocG3,flxpos,flxpo4t2s
SED(76): flxsit2s

RCA "Hot-Start" Files - RCAFIC and RCAFICSED

The RCAFIC file is used to save the "end of simulation" water column concentrations for use as initial conditions if the user chooses to perform a cycled (or "hot-start") run, while the RCAFICSED file contains similar information but for the sediment nutrient flux model (if used).

RCAFIC (internal RCA file number 15)
Record 1: CARAY
where CARAY an array (NX x NY x NZ x NOSYS) containing the concentrations for each model segment/system in the model domain (NX x NY x NZ) for each water quality variable (NOSYS) (Real)

RCAFICSED (internal RCA file number 16)
Record 1: CTEMP, CPOP, CPON, CPOC, CPOS, PO4T2, NH4T2, NO3T2, H2ST2, SIT2, BNTHSTRS, PO4T1, NH4T1, NO3T1, SIT1, H2ST1, CH4T1, CH4T2, SO4T2, PO41, NH41, NO31, H2S1, SI1, O2O, SOD, DDO, BFORMAXS, ISWBNTHS
where "array" are arrays (NX x NY x NZ), as listed above, containing the sediment bed concentrations, benthic stress, SOD, overlying water column, depth of aerobic layer for each sediment model segment (Real)

RCA Flux Balance/Mass Balance Files - RCAFMB and RCAMBSED

Should the user chose to perform flux balance/mass balance computations for an RCA simulation, the requested information will be written to RCAFMB for the water column and RCAMBSED for the sediment nutrient flux model if it is used in the model computations.

RCAFMB (internal RCA file number 17)
Records 1 -> TIME,SYSMASS,SYSLOADS,FLXMB,FLYMB
where TIME is the time at which the flux balance/mass balance computations are being written,
SYSMASS a vector (NOSYS) containing the total mass for each system in the model(Real).

SYSLOADS	an array (4,NOSYS) containing the total mass loading rate (g/day) for each system in the model. These loading rates are point source, nonpoint source, fall-line, and atmospheric, respectively.
FLXMB	an array (NX x NY) containing the depth-integrated flux terms (mg/day) for each X-interface in the model
FLYMB	an array (NX x NY) containing the depth-integrated flux terms (mg/day) for each Y-interface in the model

Record 1 contains the mass balance/flux balance terms at the start of the mass balance/flux balance computations, while records 2 and forward contain the same computations written at an interval selected by the user.

<u>RCAFMBSED (internal RCA file number 18)</u>

Records 1 -> TIME, TOTORGP, TOTORGN, TOTORGC, TOTBSI, TOTPO4, TOTNH4, TOTNO3, TOTSI, TOTH2S, TOTCH4, TOTSO4, JPOP, JPON, JPOC, JBSI, JPO4SS, JSISS, BURIALORGP, BURIALORGN, BURIALORGC, BURIALBSI, BURIALPO4, BURIALNH4, BURIALNO3, BURIALSI, BURIALH2S, BURIALCH4, BURIALSO4, TOTJPO4, TOTJN4, TOTNHO3, TOTHN2, TOTJSI, TOTJH2S, TOTJCH4AQ, TOTHCH4G, TOTSOD

where TIME	is the time at which the flux balance/mass balance computations are being written,
"arrays"	arrays (NX x NY) containing the total mass or flux rate, as listed above, for each relevant system of the sediment flux model (Real).

Record 1 contains the mass balance/flux balance terms at the start of the mass balance/flux balance computations, while records 2 and forward contain the same computations written at an interval selected by the user.

<u>Internal RCA Files</u>

In addition to the files listed about, RCA utilizes a number of input files and/or temporary files for saving intermediate computations. The following file numbers are reserved by RCA for use as input files:

30 - gcm_geom, wet_grid, and the hydrodynamic transport file(s) - HYDFILNA
31 - the diffuser file (DIFFILNA) generated by the hydrodynamic model
32 - the boundary condition file (BCFILNA)
33 - the point source file (PSFILNA)
34 - the nonpoint source file (NPSFILNA)
35 - the fall-line source file (FLFILNA)
36 - the atmospheric source file (ATMFILNA)
37 - the parameters, constants, and time-variable functions input file (PCFILNA)
38 - the initial conditions file (ICFILNA).

When developing new kinetic subroutines, the model develop should be aware of the file numbers already "assigned" by RCA and should be careful not to assign "new" files to existing file numbers (i.e., 10-18 and 30-38).