Introduction

CE-QUAL-ICM was designed to be a flexible, widely-applicable eutrophication model. Initial application was to Chesapeake Bay (Cerco and Cole 1994). Subsequent additional applications included the Delaware Inland Bays (Cerco et al. 1994), Newark Bay (Cerco and Bunch 1997), the San Juan Bay Estuary (Bunch et al. 2000), and Lake Washington (Cerco and Noel 2003). Each model application employed a different combination of model features and required addition of system-specific capabilities.

The production of user's guides describing various model versions has lagged greatly. The most recent user's guide was produced in 1995 for Release 1.0 of the model (Cerco and Cole 1995). The sponsor of the Lake Washington application has requested an up-to-date manual to accompany the transfer of model code to the sponsor. Production of a guide for this "real world" application presents a dilemma. On one hand, the guide should be a general description of the model. On the other hand, the guide must describe specific features of the Lake Washington application. The original guide was distributed with a thirty-box demonstration model. Set up of the thirty-box model was easily described and model input files could be included in their entirety in the text. Set up of the Lake Washington application is much more complex and the large input files cannot be completely listed in this guide. For economy of space, we have occasionally retained examples from the thirty-box model. In other cases, we have truncated Lake Washington files to presentable size. We endeavor to be general in the description of the model while explicitly listing instances in which the application differs from the basic examples presented here.

Model Features

Features of the model include:

Operational in one- two- or three-dimensional configurations.

Twenty-seven state variables including physical properties; multiple forms of algae, zooplankton, carbon, nitrogen, phosphorus, and silica; dissolved oxygen; and a pathogen and two toxicants.

Living resources including submerged aquatic vegetation, benthic filter feeders, and benthic deposit feeders.

Sediment-water oxygen and nutrient fluxes may be computed in a predictive submodel or specified based on observations.

State variables may be individually activated or deactivated.

Internal averaging of model output over arbitrary intervals.
Computation and reporting of concentrations, mass transport, kinetics transformations, and mass balances.

Debugging aids include ability to activate or deactivate model features, diagnostic output, volumetric and mass balances.

Coded in ANSI Standard FORTRAN F77.

Model Limitations

The model does not compute hydrodynamics. Flows, diffusion coefficients, and volumes must be specified externally and read into the model. Hydrodynamics may be specified in binary or ASCII format. Hydrodynamics are usually obtained from a hydrodynamics model such as the CH3D-WES model (Johnson et al. 1991). Information on coupling to CH3D-WES is provided in an appendix to this manual.

The user must provide processors that prepare input files and process output for presentation.

Model Structure

The model consists of a main program, an INCLUDE file, and subroutines. Both main program and subroutines perform read and write operations on numerous input and output files.

Model Programs and Subprograms

Program MAIN

The main program has three primary functions that occupy sequential sections of the program. The first function includes setting specifications for the model run and opening input and output files. The second function is solution of the three-dimensional mass-balance equation. The third function is processing of desired output and writing the output to designated files.

The INCLUDE File

The INCLUDE file contains specification and DIMENSION statements for variables held in COMMON. A key feature of the INCLUDE file is a PARAMETER statement that sets dimensions for most variables. The INCLUDE file is incorporated in the MAIN program and subroutines through the FORTRAN "INCLUDE" statement.

Subroutine TVDS

Subroutine TVDS reads time-variable information from designated input files. Files are initially opened in program MAIN. Subsequent OPEN and CLOSE operations are performed in subroutine TVDS.

Subroutine HYDRO

Subroutine HYDRO reads hydrodynamics information from designated input files. Files are initially opened in program MAIN. Subsequent OPEN and CLOSE operations are performed in subroutine HYDRO.

Subroutine AVERAGES

Subroutine AVERAGES performs temporal averaging on quantities computed internally by the model. The averaged information is written to designated files, at user-specified intervals, by program MAIN.

Subroutines ALG_READ, ALGAE

Subroutine ALG_READ reads the parameter values used to compute algal kinetics and prints them to an output file. Kinetics and settling for multiple algal groups are computed in subroutine ALGAE. Algal settling and kinetics are supplied to the mass-balance equations for the algal groups in program MAIN.

Subroutine TEMPER

Subroutine TEMPER computes heat transfer through the water surface. The transfer rate is incorporated in the transport equation for temperature in program MAIN.

Subroutine SOLIDS

Subroutine SOLIDS computes the settling of inorganic solids through the water column. Settling computed explicitly in this subroutine is supplied to the mass-balance equation for solids in program MAIN. Settling of solids (and all other variables) is treated explicitly so that settling rate can be varied independently of the externally-computed hydrodynamics.

Subroutines ZOO_READ, ZOOPL

Subroutine ZOO_READ reads the parameter values used to compute zooplankton kinetics and prints them to an output file. Kinetics for two zooplankton groups are computed in subroutine ZOOPL. Zooplankton kinetics are supplied to the mass-balance equations for the zooplankton in program MAIN.

Subroutine CARBON

Kinetic sources and sinks of carbon and settling of the particulate forms are computed in subroutine CARBON. Settling and kinetics are supplied to the mass-balance equations for carbon species in program MAIN.

Subroutine NITROG

Kinetic sources and sinks of nitrogen and settling of the particulate forms are computed in subroutine NITROG. Settling and kinetics are supplied to the mass-balance equations for nitrogen species in program MAIN.

Subroutine PHOSP

Kinetic sources and sinks of phosphorus and settling of the particulate forms are computed in subroutine PHOSP. Settling and kinetics are supplied to the mass-balance equations for phosphorus species in program MAIN.

Subroutine CODMND

Kinetic sources and sinks of chemical oxygen demand are computed in subroutine CODMND. Kinetics are supplied to the mass-balance equation for chemical oxygen demand in program MAIN.

Subroutine OXYGEN

Kinetic sources and sinks of dissolved oxygen are computed in subroutine OXYGEN. Kinetics are supplied to the mass-balance equation for dissolved oxygen in program MAIN.

Subroutine SILICA

Kinetic sources and sinks of silica and settling of the particulate form are computed in subroutine SILICA. Settling and kinetics are supplied to the mass-balance equations for silica species in program MAIN.

Subroutine BEN_FLUX

Subroutine BEN_FLUX computes sediment-water fluxes of dissolved oxygen and nutrients as functions of temperature and other conditions in the water column. Specification of benthic fluxes is an alternative to employment of the fully-predictive sediment submodel. Fluxes computed in subroutine BEN_FLUX are provided to kinetics subroutines. From the kinetics subroutines, the fluxes are supplied to appropriate mass-balance equations in program MAIN.

Subroutine PTT_READ

Subroutine PTT_READ reads the parameter values used to compute kinetics for a pathogen and two toxicants. These are printed to an output file.

Subroutine PATHOGEN

Kinetic sources and sinks of a pathogen are computed in subroutine PATHOGEN. Kinetics are supplied to the mass-balance equation for the pathogen in program MAIN.

Subroutines TOXIC1, TOXIC2

Kinetic sources and sinks of two toxicants and settling of the particulate forms are computed individually in subroutines TOXIC1 and TOXIC2. Settling and kinetics are supplied to the mass-balance equations for toxicants in program MAIN.

Subroutines SED_TOX1, SED_TOX2

Kinetic sources and sinks of two toxicants in benthic sediments are computed individually in subroutines SED_TOX1 and SED_TOX2. Sediment-water fluxes computed in these subroutine are provided to the kinetics subroutines. From the kinetics subroutines, the fluxes are supplied to appropriate mass-balance equations in program MAIN.

Subroutine SED_READ, SED_CALC

This subroutine is the major portion of the predictive sediment submodel. The subroutine has two entry points. Input required by the sediment submodel is supplied at entry SED_READ. Calculation of concentrations and fluxes in the sediments are conducted at entry SED_CALC.

Subroutine SEDTSFNL

Subroutine SEDTSFNL provides a solution algorithm for a generalized mass-balance equation in the sediments.

Subroutines SAV_READ, SAV_COMP

Subroutine SAV_READ reads the parameter values used to compute submerged aquatic vegetation (SAV) kinetics and prints them to an output file. Kinetics for SAV are computed in subroutine SAV_COMP. Exchanges between SAV and the water column and SAV and the benthic sediments are provided to kinetics subroutines and to the predictive sediment submodel.

Subroutine SUSPFEED

Subroutine SUSPFEED computes kinetics for multiple groups of benthic filter feeders. Exchanges between filter feeders and the water column and filter feeders and the benthic sediments are provided to kinetics subroutines and to the predictive sediment submodel.

Model Input Files

The Control File

The control file is the primary input file for the water-quality model. Run specifications and names of additional input and output files are specified in the control file.

The Map File

The water-quality model operates on an "unstructured" grid. Unstructured means that model cells are not referenced in an i-j-k coordinate system. Cells are located, relative to adjacent cells, through the map file.

The Geometry File

The contents of the geometry file vary depending on the format of the hydrodynamic input. If hydrodynamics are in ASCII, the geometry file contains cell dimensions as well as supplementary mapping information. If hydrodynamics are in binary, cell dimensions are input through the hydrodynamic files and the geometry file contains supplementary mapping information only.

The Initial Conditions Input File

The initial conditions file contains concentrations of state variables, in water and sediment, at initiation of the model run. Multiple options are offered for specification of initial conditions.

The Algal Growth Rates File

The algal growth rates file contains parameter values for three algal groups. These are specified once, at initiation of the model run, and read through subroutine ALG_READ.

The Zooplankton File

The zooplankton file contains parameter values for two zooplankton groups. These are specified once, at initiation of the model run, and read through subroutine ZOO_READ.

The Suspension Feeder File

The suspension feeder file contains parameter values for multiple groups of benthic filter feeders. These are specified once, at initiation of the model run, and read through program MAIN.

The Settling Rates File

The settling rates file contains settling rates for suspended solids, algae, and detritus. These are specified once, at initiation of the model run, and read through program MAIN.

The Mineralization Rates File

The mineralization rates file contains numerous kinetics rates including organic matter hydrolysis and mineralization, nitrification, and reaeration. All are specified once, at initiation of the run, and read through program MAIN.

The Pathogen and Toxics File

The pathogen and toxics file contains parameter values for a pathogen and two toxicants groups. These are specified once, at initiation of the model run, and read through subroutine PTT_READ.

The Light Extinction File

The light extinction input file contains parameter values for computation of light extinction throughout the water column. These are specified once, at initiation of the model run, and read through program MAIN.

The Hydrodynamics File

The hydrodynamics file contains transport information used to solve the mass-balance equation. Hydrodynamics may be in binary or ASCII. Multiple hydrodynamics files may be employed. They are opened sequentially in order specified in the control file.

The Meteorological Input File

The meteorological input file contains information required to compute surface heat transfer. The file also contains surface irradiance, employed in computation of algal growth, and windspeed, used to compute reaeration. Multiple files may be employed. They are opened sequentially in order specified in the control file.

The External Loads Files

The external loads files contain location and magnitude of mass loading of state variables. These loads represent point-source loads, distributed nonpoint source loads, and loads from tributaries. Three load files, designated S1, S2, S3, may be opened simultaneously to allow for differentiation of source and timing of loads. Additional files may be opened sequentially in order specified in the control file.

The Atmospheric Load File

The atmospheric load file contains information necessary to compute atmospheric nutrient loads directly to the water surface. Multiple files may be employed. They are opened sequentially in order specified in the control file.

The Submerged Aquatic Vegetation File

The submerged aquatic vegetation file takes two forms. If the predictive SAV model is employed, this file contains model parameter values, input through subroutine SAV_READ. The user also has the option of explicitly specifying exchange of material between the water column and SAV beds. In that case, the submerged aquatic vegetation file contains information on bed area and exchange rates. Multiple files may be employed. They are opened sequentially in order specified in the control file.

The Constituent Boundary Conditions File

The constituent boundary conditions file contains concentrations of state variables specified at open boundaries. Multiple files may be employed. They are opened sequentially in order specified in the control file.

The Benthic Flux Input File

The contents of the benthic flux input file vary depending on the option selected for benthic fluxes. If fluxes are predicted through the sediment submodel, the file contains input to the submodel. Otherwise, the file contains user-specified fluxes and parameters that specify effects of temperature and other influences. Multiple files may be employed. They are opened sequentially in order specified in the control file.

Model Output Files

The Initial Conditions Output File

Computed concentrations at the end of a model run can be written, in binary, to the initial conditions output file. This file can be used, with no modification, as an initial conditions input file in a subsequent model run.

The Snapshot File

The snapshot file is the primary ASCII output file. The first portion of the file is a listing of run specifications and files named in the control file. The remainder of the file is devoted to printouts of state-variable concentrations in the water and sediments. Printouts occur at user-specified intervals.

The Restart Output File

The restart output file contains the same information as the binary initial conditions file. Multiple restart output files may be created at user-specified intervals. The restart output file may be used as an initial conditions file in a subsequent model run. In the event of a model failure, the restart output file provides opportunity to restart the run near the time when it failed. This file does not, however, provide all information required for a complete “hot start.”

The Plot File

Instantaneous values of quantities computed by the model are written in binary to the plot file. Up to four groups are provided according to user specifications. The first group contains state variable concentrations in the water column. The second group contains information on algal processes and limitations. The third group contains concentrations in the sediment and sediment-water fluxes. The fourth group contains quantities computed by the SAV submodel. Quantities are written to the plot file at user-specified intervals.

The user must supply a postprocessor to view and analyze information contained in the plot file.

The Average Plot File

The average plot file contains the same quantities and provides the same options as the plot file. Quantities written to the average plot file are temporally averaged over user-specified intervals, however. The average plot file is useful for determining daily or seasonal averages of model computations. The user must supply a postprocessor to view and analyze information contained in the average plot file.

The Diagnostic File

The diagnostic file is an ASCII file that provides information useful in interpreting and debugging model runs. Diagnostic information includes volume and mass balances, timestep and stability limitations, and a record of input files opened. Diagnostic information is available at user-specified intervals.

The Transport Flux File

The transport flux file contains, in binary form, computed transport of a subset of state variables across the interfaces of model cells. Transport fluxes are averaged at user-specified intervals and output in binary form for each cell in the grid. The user must supply a postprocessor to view and analyze information contained in the transport flux file.

The Kinetics Flux File

Kinetic transformations of state variables occur through a variety of pathways. Transformation rates through individual processes are tracked in the model. Transformations are averaged at user-specified intervals and output in binary form for each cell in the grid. The user must supply a postprocessor to view and analyze information contained in the kinetics flux file.

The Oxygen Volume File

The oxygen volume file provides an accounting of volume and duration of water within user-specified limits of dissolved oxygen concentration. The accounting is useful to determine volume and duration of anoxia, for example. Oxygen volumes are averaged at user-specified intervals and output in binary form for each cell in the grid. The user must supply a postprocessor to view and analyze information contained in the oxygen volume file.

The Mass-Balance File

The mass-balance file reports net addition or removal of carbon, nitrogen, and phosphorus from each cell. Processes included in the mass-balance accounting are external loads, atmospheric loads, benthic fluxes, burial, and internal sources/sinks. Mass balances are averaged at user-specified intervals and output in binary form for each cell in the grid. The user must supply a

postprocessor to view and analyze information contained in the mass-balance file. The mass-balance file does not contain the system-wide mass accounting provided in the diagnostic file.

The Algal Output File

The algal output file contains, in ASCII format, the algal kinetics parameters reported by subroutine ALG_READ.

The Zooplankton Output File

The zooplankton output file contains, in ASCII format, the zooplankton kinetics parameters reported by subroutine ZOO_READ.

The Benthic Flux Output File

The benthic flux output file provides an ASCII listing of information input to the sediment submodel. In the event user-specified fluxes are employed, this file reports the fluxes.

The SAV Output File

The SAV output file contains, in ASCII format, the submerged aquatic vegetation kinetics parameters reported by subroutine SAV_READ.

The Suspension Feeder Output File

The suspension feeder output file reports, in binary form, diagnostic information from the benthic filter feeder submodel. The user must supply a postprocessor to view and analyze information contained in this file.

The Pathogen and Toxics Output File

The pathogen and toxics output file contains, in ASCII format, kinetics parameters for pathogens and toxics reported by subroutine PTT_READ.

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The Conservation-of-Mass Equation

The Model Grid

Application of the model requires division of the study system into a grid of discrete volumes or cells. Although each volume is three-dimensional, the grid may be one-, two-, or three-dimensional, depending on the arrangement of the cells. An example of a two-dimensional grid is shown as Figure 1. This grid contains ten cells in the longitudinal dimension, one cell in the lateral dimension, and three cells in the vertical dimension.

Each cell in the grid is assigned a unique number or index (Figure 2). Interfaces are numbered where flows pass between cells or where cells adjoin open boundaries. Faces adjacent to solid boundaries are not numbered. The grid is unstructured. That is, the cell indices contain no information that indicates cell location in a three-dimensional coordinate system. Neither is there a general relationship between the indices of adjacent cells or between cells and flow faces. A connectivity or "map" file is required that locates cells and faces relative to each other.

The unstructured grid of discrete volumes provides maximum flexibility in coupling the water-quality model with hydrodynamic models. No restriction is placed on cell shape or number of flow faces per cell. A price is paid for the flexibility, however. Model coding is more complex for the unstructured grid than for a structured grid. Creation of the map file and coupling with a hydrodynamic model that operates on a structured grid are time-consuming, exacting tasks. The procedure for coupling the eutrophication model with the structured CH3D-WES hydrodynamic model is described in an appendix to this manual.

The Conservation-of-Mass Equation

The foundation of CE-QUAL-ICM is the solution to the three-dimensional mass-conservation equation for a control volume. CE-QUAL-ICM solves, for each volume and for each state variable, the equation:

$$\frac{\delta V_j C_j}{\delta t} = \sum_{k=1}^{n} Q_k C_k + \sum_{k=1}^{n} A_k D_k \frac{\delta C}{\delta x_k} + \sum S_j \qquad (1)$$

V_j = volume of jth control volume (m^3)
C_j = concentration in jth control volume (gm m^{-3})
Q_k = volumetric flow across flow face k of jth control volume (m^3 sec^{-1})
C_k = concentration in flow across flow face k (gm m^{-3})
A_k = area of flow face k (m^2)
D_k = diffusion coefficient at flow face k (m^2 sec^{-1})
n = number of flow faces attached to jth control volume
S_j = external loads and kinetic sources and sinks in ith control volume (gm sec^{-1})
t, x = temporal and spatial coordinates

Discretization of the Conservation Equation

Solution of the conservation-of-mass equation on a digital computer requires specification of parameter values and discretization of the continuous derivatives. Numerous formulae for evaluation and discretization exist. Formulae employed in CE-QUAL-ICM were selected based on computational efficiency and accuracy.

The conservation-of-mass equation is solved in two steps. In the first step, an intermediate value is computed. The intermediate value includes the effects of change in cell volume, longitudinal and lateral transport, and external loading. In the second step, the effects of vertical transport are computed.

Longitudinal and Lateral Advection

Solution to the conservation-of-mass equation in the longitudinal and lateral directions is via explicit time stepping. That is:

$$C_j^* = \frac{V_j}{V_j^{t+\Delta t}} C_j + \frac{\Delta t}{V_j^{t+\Delta t}} \left(\sum_{k=1}^{nhf} Q_k C_k + \sum_{k=1}^{nhf} A_k D_k \frac{\delta C}{\delta x_k} + \sum S_j \right) \qquad (2)$$

C_j^* = concentration in jth control volume after volume change, loading, longitudinal/lateral transport processes
$V_j^{t+\Delta t}$ = volume of jth control volume at time t=Δt
Δt = discrete time step
nhf = number of longitudinal and lateral flow faces attached to jth control volume

The remaining parameters in Equation 2 are evaluated at time t.

Upwind Differencing. Solution of Equation 2 requires evaluation of the C_k. Two options are provided within CE-QUAL-ICM. The first is backwards or upwind differencing. In upwind differencing, concentration in the flow across any face is taken as concentration in the cell upstream of the face (Figure 3). Upstream is defined relative to direction of the flow. Upstream has no relation to the cell coordinate system.

QUICKEST. A second approximation to C_k fits a parabola to concentration in three adjacent cells (Figure 3). For uniform grid spacing:

$$C_k = \frac{1}{2}\left(C_i + C_j\right) - \frac{1}{8}\left(C_{il} + C_j - 2\ C_i\right) \qquad (3)$$

The approximation in Equation 3 is the basis of the QUICK (Quadratic Upstream Interpolation for Convective Kinematics) method. An extension of QUICK for unsteady flows, QUICKEST (QUICK with Estimated Streaming Terms) is implemented in the model. Details of QUICK and QUICKEST, including the QUICKEST formulae for unsteady flows on a non-uniform grid, are provided by Leonard (1979).

Upwind differencing provides computational simplicity. The upwind method is less accurate and less stable than QUICKEST, however. The primary disadvantage of QUICKEST is that the method sometimes generates negative concentrations when advecting sharp concentration gradients. A second disadvantage is that QUICKEST cannot be implemented on highly-irregular grids (e.g. finite element grids) in which two upstream cells cannot be readily identified.

Detailed knowledge of the advective solution schemes are not necessary to execute the model. The upwind and QUICKEST approximations were reviewed to indicate the information required by the model to compute advective transport in the longitudinal and lateral directions. To compute advective transport in any cell, the model requires:

Cell volume.

Indices of longitudinal and lateral flow faces adjoining the cell.

Indices of adjoining and next-most adjoining cells.

Volumetric flow across the indexed flow faces.

Length of indexed cells.

The required information is provided in the map, geometry, and hydrodynamics files. Formats of these files are detailed in subsequent chapters.

Longitudinal and Lateral Dispersion

Computation of longitudinal and lateral dispersion requires discrete approximation of the continuous derivative in the dispersion term of Equation 2. The basic approximation is:

$$\frac{\delta C}{\delta x_k} = \frac{C_j - C_i}{\Delta x} \tag{4}$$

Δx = distance between centers of two cells

A higher-order correction to the basic expression is computed when the QUICKEST scheme is employed.

Computation of longitudinal and lateral dispersion requires enumeration of the dispersion coefficient at each flow face. No indexing information is required beyond that supplied for the advection terms.

Vertical Transport

Solution to the conservation-of-mass equation in the longitudinal and lateral directions is by an explicit method. That is, all parameters in the discretized equation are evaluated at time t except the unknown C^*. The explicit method is suited for transport dominated by advection rather than diffusion or dispersion. In the vertical direction, diffusion is a significant or dominant component of transport. Solution of vertical transport by an explicit method requires a small time step and consumes large amounts of computer time. In CE-QUAL-ICM, solution to vertical transport is by a partly- or fully-implicit scheme that practically frees the computation from stability conditions imposed by vertical transport.

The mass-conservation equation in the vertical direction (Figure 4) can be expressed:

$$\frac{C_j^{t+\Delta t} - C_j^*}{\Delta t} = \tag{5}$$

$$(1-\theta) \sum_{k=1}^{nvf} \frac{Q_k \; C_k}{V_k} + \theta \sum_{k=1}^{nvf} \frac{Q_k^{t+\Delta t} \; C_k^{t+\Delta t}}{V_k^{t+\Delta t}} + \sum_{k=1}^{nvf} \frac{A_k \; D_k}{V_k^{t+\Delta t}} \; \frac{\delta C^{t+\Delta t}}{\delta z}$$

θ = implicit weighting factor ($0 \le \theta \le 1$)
nvf = number of vertical faces

z = vertical coordinate

The implicit weighting factor, θ, determines whether vertical advection is computed explicitly (θ = 0), implicitly (θ = 1), or is weighted between the two extremes (0 < θ < 1). Computational stability is enhanced as θ --> 1, at the expense of increased numerical diffusion. The value θ = 0.75 is recommended.

Since vertical velocities are usually much less than longitudinal velocities, the enhanced accuracy of the QUICKEST scheme is not necessary. The values of C_k and $C_k^{t+\Delta t}$ are computed by linear interpolation (Figure 4) between concentrations at the centers of adjoining cells:

$$C_k = \frac{C_i \ \Delta z_i + C_j \ \Delta z_j}{\Delta z_i + \Delta z_j} \tag{6}$$

The spatial gradient in the diffusion term is evaluated by central difference (Equation 4) evaluated at time step t+Δt.

The solution scheme for vertical transport is an implicit scheme which means that the equation for concentration in any cell at time t+Δt (e.g. Equation 5) contains multiple unknowns. Computation of concentration in any one cell requires solution of a set of simultaneous equations for concentrations in a column of cells extending from water surface to bottom. Details of the solution scheme are not necessary to operate the model. The user must provide, however, the following information required to compute vertical transport:

Indices of all cells in a column.

Indices of vertical flow faces adjoining all cells in a column.

Volumes of all cells in a column.

Volumetric flow across the indexed flow faces.

Diffusion coefficients at indexed flow faces.

Length of indexed cells.

The required information is provided in the map, geometry, and hydrodynamics files. Formats of these files are detailed in subsequent chapters.

Summary of Numerical Solution Scheme

The model solves the conservation-of-mass equation through a step-by-step procedure:

1) Evaluate internal sources and sinks. These include kinetics transformations and sediment-water fluxes. This step provides a partial computation of ΣS_j in Equation 1.

2) Add effects of external loads. This step completes computation of ΣS_j in Equation 1.

3) Compute longitudinal and lateral advection and diffusion at all interfaces. This step provides quantities required to solve Equation 2.

4) Compute concentration at time $t+\Delta t$ in all cells resulting from volume changes, kinetics, external loads, and longitudinal/lateral transport. This step is the solution to Equation 2. For one- or two-dimensional (longitudinal/lateral) systems, solution of the conservation-of-mass equation is complete at this point. For two- (longitudinal/ vertical) or three-dimensional systems, the result is an intermediate solution prior to computation of vertical transport.

5) Compute vertical transport from surface to bottom. Computation is by columns. Each cell at the water surface represents the top of one column.

Water-Quality Model Time Step

Temporal integration of the conservation-of-mass equation (1) is accomplished in discrete time steps Δt (Equations 2, 5). Integration in discrete steps provides an approximation to the continuous solution of the original differential equation. As Δt --> 0, the solution of the approximate equation converges on the solution of the continuous equation, although at great cost in computation time. As Δt --> □, computation time diminishes but the solution of the discrete equation diverges from solution of the continuous equation. For sufficiently large Δt, the numerical solution may exhibit large oscillations or instabilities that produce computational failures. The occurrence of instabilities is prevalent in explicit rather than implicit solution schemes. Typical practice in numerical modeling is to select the largest time step possible, to minimize computation time, while remaining in predefined stability limits.

Vertical Transport

The implicit algorithm employed to compute transport in the vertical direction is stable for time step of any size when $\theta \geq 0.5$ (Roache 1972). Consequently, vertical transport is not considered in determination of the time step.

Longitudinal and Lateral Transport

Transport in the longitudinal and lateral directions is computed by explicit

schemes that are subject to instabilities for large Δt. The time step employed is determined by an "autostepping" algorithm. The algorithm computes permissible time step based on flow, dispersion, and cell dimension. As a consequence of autostepping, the time step varies throughout a model run. The time step is always near the maximum permissible time step. Autostepping minimizes computation time while meeting stability requirements.

Upwind Differencing. The stability requirement for explicit solution to the one-dimensional mass-conservation equation, employing upwind differencing for the advective term, is (Leonard 1979):

$$\Delta t \leq \frac{1}{\frac{2\ D}{\Delta x^2} + \frac{u}{\Delta x}} \tag{7}$$

Δt = time step (T)
Δx = cell length (L)
u = velocity ($L\ T^{-1}$)
D = diffusion coefficient ($L^2\ T^{-1}$)

The autostepping algorithm examines velocity, diffusion, and cell length (equivalent to Q_j / A_j, D_j, and δx_j in Equation 2) at each flow face of the water-quality model control volumes. Allowable time step is computed at each face. The flow face with the most restrictive time step determines the time step for the entire system. The time step is set at a user-specified fraction, α, of the maximum allowed.

QUICKEST. Inspection of the stability region of the one-dimensional QUICKEST algorithm (Leonard 1979) indicates sufficient conditions are:

$$\Delta t \leq \frac{\Delta x}{u} \tag{8}$$

and

$$\Delta t \leq \frac{\Delta x^2}{2\ D} \tag{9}$$

The autostepping algorithm examines velocity, diffusion, and cell length at each flow face of the water quality model control volumes. Allowable time step at each face is determined as:

$$\Delta t = \text{minimum}\left(\alpha\ \frac{\Delta x}{u}, \alpha\ \frac{\Delta x^2}{2\ D} \right) \tag{10}$$

α = constant that insures time step is less than maximum allowed (0.95)

The flow face with the most restrictive time step determines the time step for the entire system.

The model stability requirements for the QUICKEST algorithm are less restrictive than the stability requirements for upwind differencing. As a consequence, time steps are larger and computation time is reduced when the user specifies QUICKEST rather than upwind differencing. The model stability requirements for QUICKEST also provide a conservative evaluation of the time step. The actual stability region for QUICKEST (Leonard 1979) extends beyond the region employed in the model.

The criteria expressed in Equations 7 and 10 are for one-dimensional solutions to the mass-conservation equation. Stability requirements for two-dimensional solutions differ from requirements for one-dimensional solutions. The unstructured grid and the solution algorithms employed in the model greatly complicate application of two-dimensional criteria. We have thus far found application of the one-dimensional criteria at all flow faces is sufficient to determine the time step in multi-dimensional applications.

Boundary Conditions

Boundary conditions must be specified at the flow faces along the edges of the grid. Through these faces, material is exchanged with the environment outside the model domain. Boundary flow faces are allowed only at the longitudinal and lateral limits of the grid. No flow is allowed through the surface and bottom. Cell faces at the water surface and bottom are not indexed. Neither are cell faces indexed along longitudinal and lateral edges of the grid through which flow does not occur.

Treatment of open boundary conditions requires selection of the numerical scheme and specification of concentration in the environment beyond the grid.

Numerical Treatment

Open boundaries are specified as "left-flow boundaries" or "right-flow boundaries" (Figure 5). Left- and right-flow boundaries are defined according to the cell numbering scheme in the map file. The designation is independent of flow direction, which may be into or out of the grid.

The model employs upwind differencing at all flow boundaries. Upwind differencing occurs whether or not the QUICKEST scheme is specified for advection within the interior of the grid. Upwind differencing is appropriate treatment for inflows that occur at estuarine fall lines and at tributary entry points. Upwind differencing ensures that the concentration of flow entering the grid is the specified boundary concentration. If QUICKEST were employed at an inflow boundary, the three-point weighting scheme would compute an

influence of concentration within the system on concentration entering the system.

Upwind differencing is also employed at outflow boundaries. Employment of upwind differencing means that concentration in flow leaving the system is not influenced by concentrations outside the system. Upwind differencing exactly simulates conditions at an outflow such as a spillway. An advantage of upwind differencing at outflows is that the user need not specify a concentration outside the model domain.

Longitudinal and lateral dispersion are set to zero at inflow and outflow boundaries. Absence of dispersion is appropriate at inflow locations such as fall lines and tributary entry points. Absence of dispersion at outflows frees the user from specification of concentration outside the model domain.

Concentration in Inflows

Concentration in flow entering the system across open boundaries must be provided to the model. In most cases, such as fall lines and tributary entry points, the concentration is specified by the user.

Concentration in Outflows

Concentration in flow leaving the system across open boundaries is specified by the model as the concentration in the cell adjoining the boundary. No user specification of concentration is required.

Timing

User-specified boundary concentrations may be updated at arbitrary times during a model run. Two options are available for specification of boundary concentrations between updates (Figure 6). If the "step-function" option is selected, boundary concentrations are immediately assume the updated concentration and remain constant until the next update. If the "interpolate" option is selected, boundary concentrations are linearly interpolated between updates.

References

Leonard, B. (1979). “A stable and accurate convection modelling procedure based on quadratic upstream interpolation,” *Computer Methods in Applied Mechanics and Engineering,* 19, 59-98.

Roache, P. (1972). *Computational fluid dynamics*. Hermosa Publishers, Albuquerque NM.

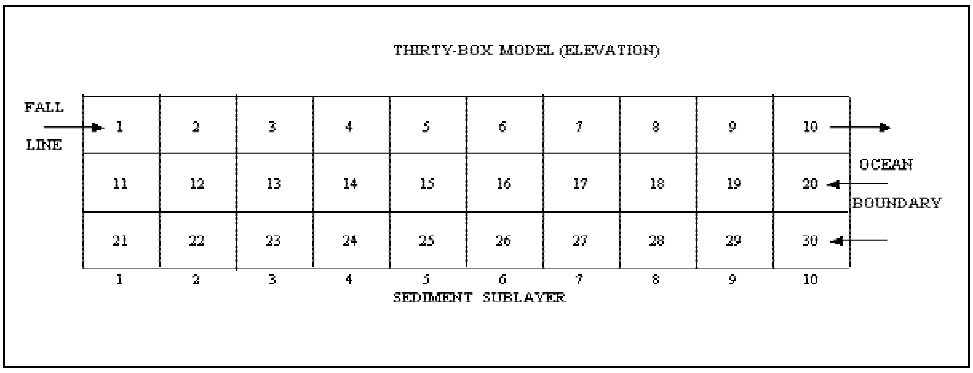

Figure 1. Two-dimensional model grid (elevation)

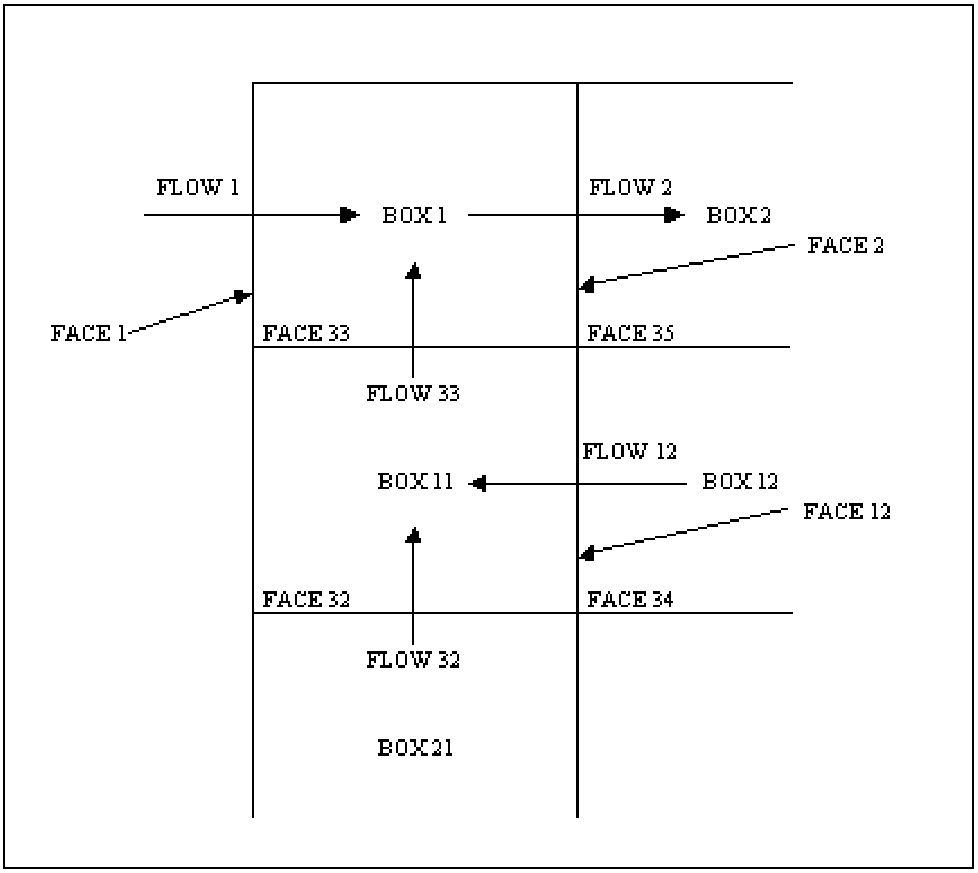

Figure 2. Cell and interface numbering scheme

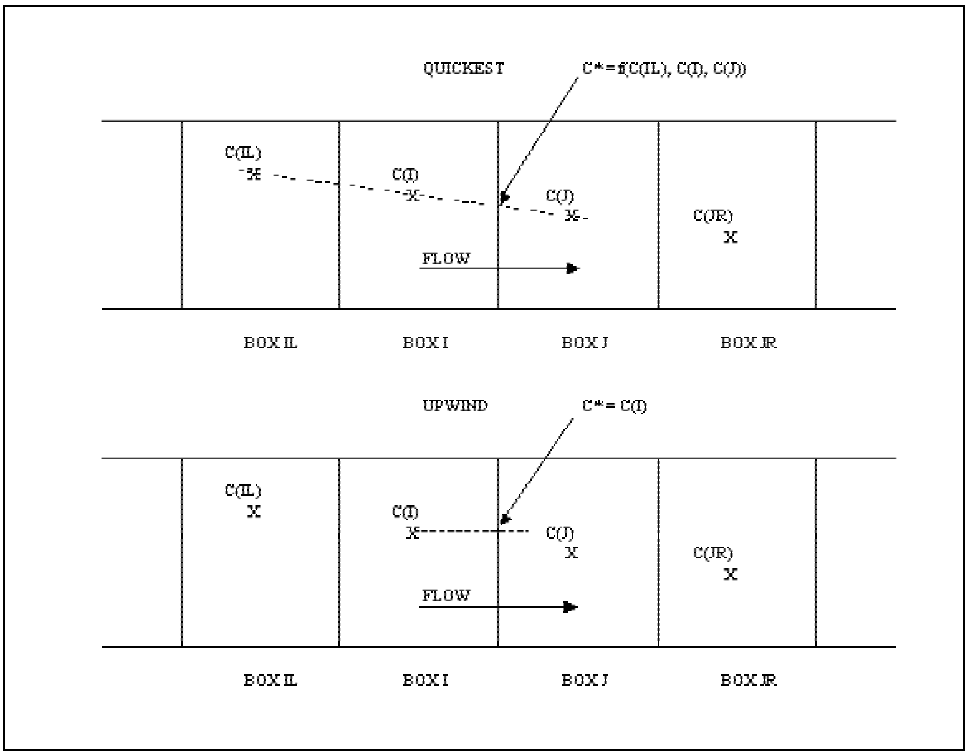

Figure 3. Upwind and QUICK advection schemes

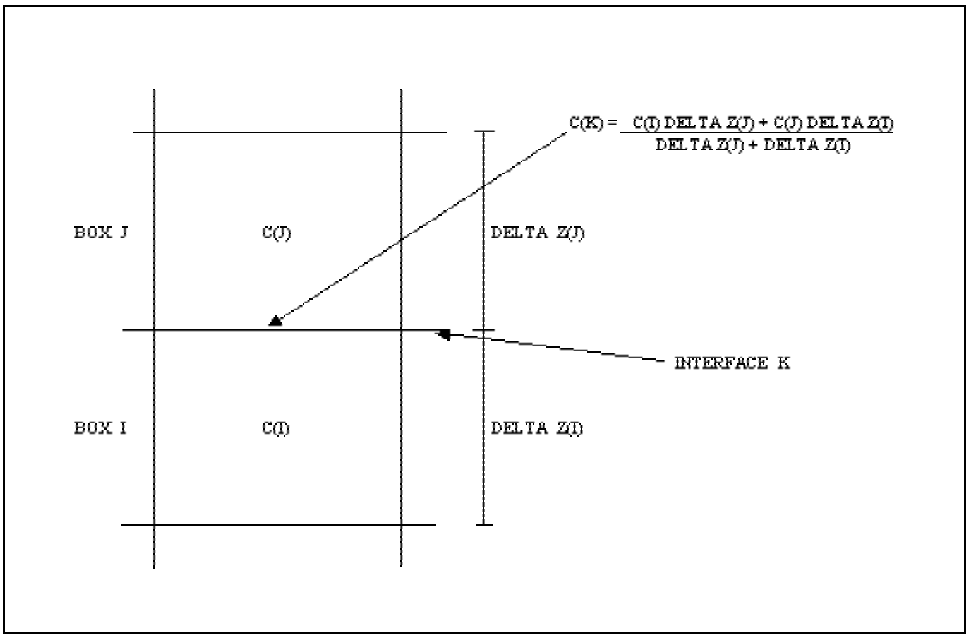

Figure 4. Vertical advection scheme

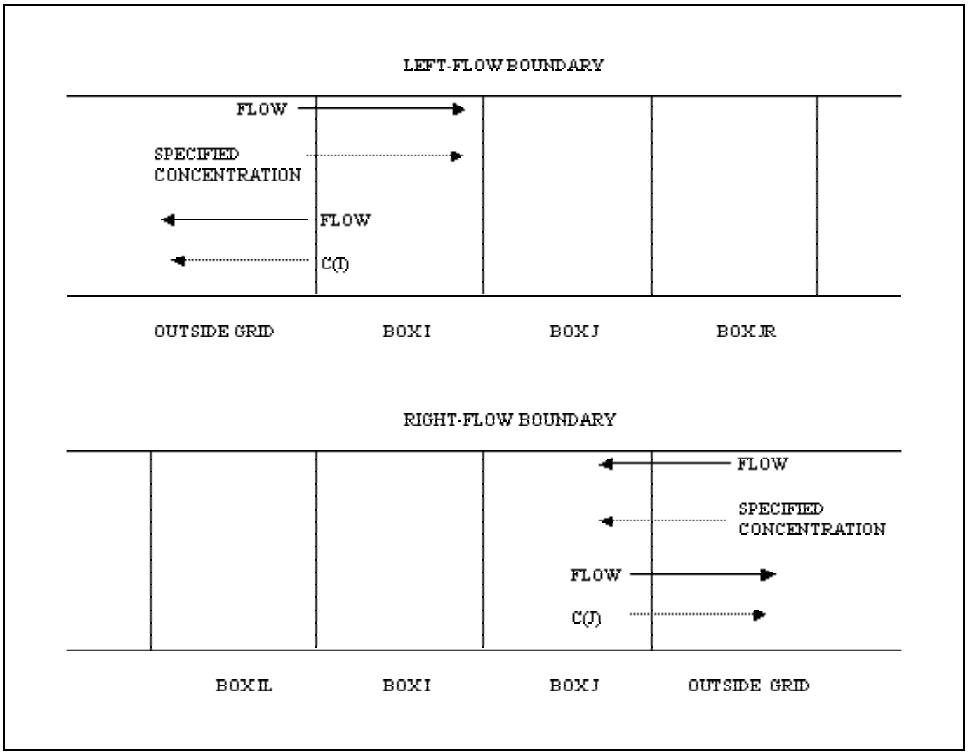

Figure 5. Left- and right-flow boundaries

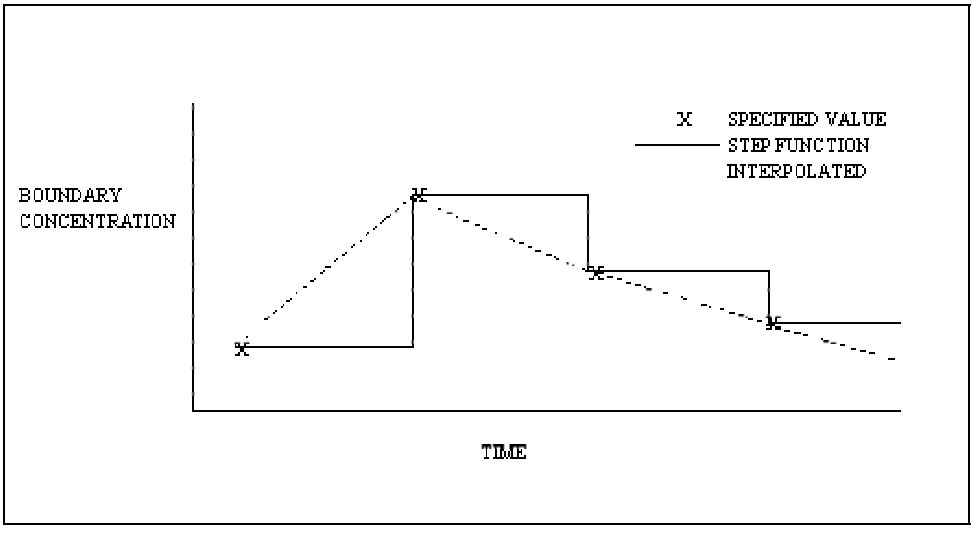

Figure 6. Step-function and interpolated boundary conditions

The Control File

The control file contains the parameters used to run CE-QUAL-ICM. It consists of card images 80 characters in length. The format of the input files has been developed in order to take advantage of a full-screen text editor. The control file begins with six lines, which can be used for file identification and are ignored by the program. The rest of the file consists of a line, which contains the card identification and the names of the FORTRAN variables associated with the input card. The FORTRAN names are right-justified according to the field widths associated with the input variable. The next line consists of the actual input values. There are 10 input fields associated with each card although the first field is not used. Each field has a length of eight characters. The next line is left blank for ease of display in a full-screen editor.

There are **no** optional cards in the control file - **each card is required** although there may be no values associated with the card. The following pages contain a description of each card. **All character inputs must be capitalized except the TITLE cards** or the variable will take on the **default** value.

Title Cards (TITLE)

Field	Name	Value	Description
1-72	TITLE	Character	Text for identification of simulation

There are six title cards that help identify the model run. Each line contains up to 72 characters of text. The title cards appear in every output file except for restarts. Uses for the title cards include identifying the application, the dates of the application, the date of the simulation, and any other information specific to the simulation.

EXAMPLE

```
TITLE C
.....................................Title.....................................
        Start revisions of Lake Washington model
        Fix-ups first, then major revisions
        Run from /disk3/cerco/lake_wash
        February 25, 2001
        Mass balance and Sensitivity runs of 30-box 3-D grid.
        Initial code from /cc1/cerco/SENS43_new_grid (Ches Bay)
```

Geometry Definition (GEOM DEFINE)

Field	Name	Value	Description
1	NB	Integer	Number of boxes in grid
2	NSB	Integer	Number of surface boxes in grid
3	NQF	Integer	Number of flow faces in grid
4	NHQF	Integer	Number of horizontal flow faces in grid
5	NSHQF	Integer	Number of horizontal flow faces in surface layer of grid
6	NL	Integer	Maximum number of layers in grid

This card specifies the dimensions of the water-quality model grid. The user must take care that the values specified here are less than or equal to the corresponding PARAMETER statements in the file WQM_COM.INC.

EXAMPLE

```
GEOM DEFINE    NB      NSB      NQF    NHQF   NSHQF      NL
           12177      655    32869   21347    1177      41
```

Time Control (TIME CON)

Field	Name	Value	Description
1	TMSTRT	Real	Starting simulation date (Julian day)
2	TMEND	Real	Ending simulation date (Julian day)

This card specifies the starting and ending dates of the simulation.

EXAMPLE

```
TIME CON  TMSTRT   TMEND
            0.0  1095.5
```

Number of Timestep Intervals (# DLT)

Field	Name	Value	Description
1	NDLT	Integer	Number of timestep intervals

The model provides the option to vary the time step. The time step may be varied through the autostepping option or at discrete, user-specified intervals. This card specifies the number of intervals in which the timestep, maximum timestep, and/or the fraction of the calculated timestep vary.

This card group establishes a pattern followed by successive groups which govern output. The first card establishes that time steps are assigned once. The second card names the time as day 0. The third card assigns a time step of 2400 seconds at day 0.

EXAMPLE

```
# DLT       NDLT
              1
```

Timestep Date (DLT DAY)

Field	Name	Value	Description
1	DLTDAY	Real	Date of timestep interval (Julian day)

This card specifies the intervals in which the timestep, maximum timestep, and/or fraction of the maximum calculated timestep may vary.

EXAMPLE

```
DLT DAY     DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD
             0.0
```

Timestep Value (DLT VAL)

Field	Name	Value	Description
1	DLTVAL	Real	Timestep (sec)

This card specifies the initial timestep if autostepping is used or the values for the timestep if autostepping is turned off.

EXAMPLE

```
DLT VAL   DLTVAL  DLTVAL  DLTVAL  DLTVAL  DLTVAL  DLTVAL  DLTVAL  DLTVAL  DLTVAL
          2400.0
```

Maximum Timestep (DLT MAX)

Field	Name	Value	Description
1	DLTMAX	Real	Maximum timestep (sec)

This card specifies the maximum value for the timestep if autostepping is turned on.

EXAMPLE

```
DLT MAX   DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX
          2400.0
```

Timestep Fraction (DLT FTN)

Field	Name	Value	Description
1	DLTFTN	Real	Fraction of calculated timestep used

This card specifies the fraction of the timestep used if autostepping is turned on. The autostepping algorithm estimates the maximum timestep in order to maintain stability. Since this is an estimate, DLTFN can be used to decrease the timestep if the model becomes unstable when autostepping is turned on.

EXAMPLE

```
DLT FTN    DLTFTN  DLTFTN  DLTFTN  DLTFTN  DLTFTN  DLTFTN  DLTFTN  DLTFTN  DLTFTN
             0.90
```

Hydrodynamic Model Timestep (HM DLT)

Field	Name	Value	Description
1	AHMDLT	Real	Hydrodynamic update interval (sec)
2	FILGTH	Real	Ending date of hydrodynamic file (Julian day)

This card specifies the interval at which hydrodynamic information is input to the model. This information is employed only if "BINARY" or "DEPTH-AVERAGE" options are specified (see card HYD MODEL). The present formulation requires a constant update interval. The ending date of the hydrodynamic input (HMEND) is necessary to synchronize elapsed time in the model, time determined from hydrodynamic updates, and update times specified on various input files. If multiple hydrodynamic files are employed, they should be as close to one year in length as possible.

EXAMPLE

```
HM DLT     AHMDLT   HMEND
           3600.0   365.0
```

Snapshot Output Control (SNAPSHOT)

Field	Name	Value	Description
1	SNPC	Character	Specifies if output is written to snapshot file
2	NSNP	Integer	Number of snapshot intervals

This card specifies if information is output to the snapshot file. The output interval is variable. The card also lists the number of intervals in which the frequency varies.

The first card in this card group indicates that snapshot frequency is specified one time. The second card indicates frequency is specified on day 0. The final card indicates snapshots are put out at a frequency of every 365 days starting at day 0.

EXAMPLE

```
SNAPSHOT     SNPC     NSNP
               ON        1
```

Snapshot Date (SNAP DAY)

Field	Name	Value	Description
1-9	SNPD	Real	Date of snapshot interval (Julian day)

This card specifies the intervals at which the snapshot output varies. If there are more intervals than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
SNAP DAY     SNPD     SNPD     SNPD     SNPD     SNPD     SNPD     SNPD     SNPD     SNPD
               0.0
```

Snapshot Frequency (SNAP FREQ)

Field	Name	Value	Description
1-9	SNPF	Real	Snapshot output frequency (Julian day)

This card specifies the frequency at which snapshot information is output. If there are more values than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
SNAP FRQ    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF
          365.0
```

Plot Output Control (PLOT)

Field	Name	Value	Description
1	PLTC	Character	Specifies if output is written to plot file
2	QPLTC	Character	Specifies if water quality information is output
3	SPLTC	Character	Specifies if sediment information is output
4	SAVPLTC	Character	Specifies if Submerged Aquatic Vegetation information is output
5	NPLT	Integer	Number of plot intervals

This card specifies if information is output to the plot file and the number of intervals in which the frequency of the output varies.

EXAMPLE

```
PLOT         PLTC   QPLTC   SPLTC SAVPLTC    NPLT
              OFF      ON      ON     OFF       1
```

Plot Date (PLOT DAY)

Field	Name	Value	Description
1-9	PLTD	Real	Date of plot interval (Julian day)

This card specifies the intervals at which the plot output varies. If there are more intervals than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
PLOT DAY    PLTD    PLTD    PLTD    PLTD    PLTD    PLTD    PLTD    PLTD    PLTD
             0.0
```

Plot Frequency (PLOT FREQ)

Field	Name	Value	Description
1-9	PLTF	Real	Plot output frequency (Julian day)

This card specifies the frequency at which plot information is output. If there are more values than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
PLOT FREQ   PLTF    PLTF    PLTF    PLTF    PLTF    PLTF    PLTF    PLTF    PLTF
            10.0
```

Average Plot Output Control (AV PLOT)

Field	Name	Value	Description
1	APLC	Character	Specifies if output is written to average plot file
2	NAPL	Integer	Number of average plot intervals

This card specifies if information is output to the average plot file and the number of times at which averaging interval varies.

The first card in this card group indicates that averaging interval is specified once. The second card indicates the interval is specified on day 0. The final card indicates the averaging interval is 1.0 day starting at day 0.

EXAMPLE

```
AV PLOT     APLC    NAPL
              ON       1
```

Average Plot Date (AVPLT DAY)

Field	Name	Value	Description
1-9	APLD	Real	Date of average plot interval (Julian day)

This card specifies the intervals at which the average plot output varies. If there are more intervals than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
AVPLT DAY   APLD    APLD    APLD    APLD    APLD    APLD    APLD    APLD    APLD
              0.0
```

Average Plot Frequency (AVPLT FREQ)

Field	Name	Value	Description
1-9	APLF	Real	Average plot output frequency (Julian day)

This card specifies the frequency at which average plot information is output. If there are more values than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
AVPLT FREQ  APLF    APLF    APLF    APLF    APLF    APLF    APLF    APLF    APLF
              1.0
```

Transport Flux Output Control (TRAN FLUX)

Field	Name	Value	Description
1	TFLC	Character	Specifies if output is written to transport flux file
2	NTFL	Integer	Number of transport flux intervals

This card specifies if information is output to the transport flux file and the number of intervals in which the frequency of the output varies. Transport flux is averaged similar to the Average Plot file.

EXAMPLE

```
TRAN FLUX    TFLC     NTFL
              OFF        1
```

Transport Flux Date (FLUX DAY)

Field	Name	Value	Description
1-9	TFLD	Real	Date of transport flux interval (Julian day)

This card specifies the intervals at which the transport flux output varies. If there are more intervals than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
FLUX DAY     TFLD     TFLD     TFLD     TFLD     TFLD     TFLD     TFLD     TFLD     TFLD
              0.0
```

Transport Flux Frequency (FLUX FREQ)

Field	Name	Value	Description
1-9	TFLF	Real	Transport flux output frequency (Julian day)

This card specifies the frequency at which transport flux information is output. If there are more values than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
FLUX FREQ   TFLF    TFLF    TFLF    TFLF    TFLF    TFLF    TFLF    TFLF    TFLF
          91.25
```

Kinetics Flux Output Control (KIN FLUX)

Field	Name	Value	Description
1	KFLC	Character	Specifies if output is written to kinetics flux file
2	NKFL	Integer	Number of kinetics flux intervals

This card specifies if information is output to the kinetics flux file and the number of intervals in which the frequency of the output varies. Kinetics fluxes are averaged similar to the Average Plot file

EXAMPLE

```
KIN FLUX    KFLC    NKFL
             OFF       1
```

Kinetic Flux Date (FLUX DAY)

Field	Name	Value	Description
1-9	KFLD	Real	Date of kinetic flux interval (Julian day)

This card specifies the intervals at which the kinetic flux output varies. If there are more intervals than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
FLUX DAY    KFLD    KFLD    KFLD    KFLD    KFLD    KFLD    KFLD    KFLD    KFLD
             0.0
```

Kinetic Flux Frequency (FLUX FREQ)

Field	Name	Value	Description
1-9	KFLF	Real	Kinetic flux output frequency (Julian day)

This card specifies the frequency at which kinetic flux information is output. If there are more values than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
FLUX FREQ   KFLF    KFLF    KFLF    KFLF    KFLF    KFLF    KFLF    KFLF    KFLF
          30.42
```

Oxygen Plot Output Control (OXY PLOT)

Field	Name	Value	Description
1	OPLC	Character	Specifies if output is written to oxygen plot file
2	NOPL	Integer	Number of oxygen plot intervals
3	NOINT	Integer	Number of oxygen concentration intervals

This card specifies if information is output to the oxygen plot file and the number of intervals in which the frequency of the output varies. In addition, it specifies the oxygen concentration ranges used in determining oxygen volume-days. Oxygen Plot output is averaged in a manner similar to the Average Plot file.

EXAMPLE

```
OXY PLOT    OPLC    NOPL   NOINT
             OFF      42       5
```

Oxygen Intervals (OXY INT)

Field	Name	Value	Description
1-9	OINT	Real	Interval value for determining oxygen volume-days

This card specifies the concentration ranges used in determining oxygen volume-days. If there are more values than can be specified on one line, then they are continued on the next line.

In the example below with NOINT=5, the intervals would be defined as
Interval 1 -10.0 <= Dissolved Oxygen < 1.0
Interval 2 1.0 <= Dissolved Oxygen < 3.0
Interval 3 3.0 <= Dissolved Oxygen < 4.0
Interval 4 4.0 <= Dissolved Oxygen < 5.0
Interval 5 5.0 <= Dissolved Oxygen

EXAMPLE

```
OXY INT     OINT    OINT    OINT    OINT    OINT    OINT    OINT    OINT    OINT
          -10.0     1.0     3.0     4.0     5.0
```

Oxygen Plot Date (OXY DAY)

Field	Name	Value	Description
1-9	OPLD	Real	Date of oxygen plot interval (Julian day)

This card specifies the intervals at which the oxygen plot output varies. If there are more intervals than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
OXY DAY     OPLD    OPLD    OPLD    OPLD    OPLD    OPLD    OPLD    OPLD    OPLD
            0.0    50.0   141.0   233.0   324.0   415.0   507.0   598.0   689.0
          780.0   872.0   963.0  1054.0  1145.0  1237.0  1328.0  1419.0  1510.0
         1602.0  1693.0  1784.0  1875.0  1967.0  2058.0  2149.0  2240.0  2332.0
         2423.0  2514.0  2605.0  2697.0  2788.0  2879.0  2971.0  3062.0  3153.0
         3244.0  3336.0  3427.0  3518.0  3609.0  3650.0
```

Oxygen Plot Frequency (OXY FREQ)

Field	Name	Value	Description
1-9	OPLF	Real	Oxygen plot output frequency (Julian day)

This card specifies the frequency at which oxygen plot information is output. If there are more values than can be specified on one line, then they are continued on the next line.

In the example below, the 365.0 day frequency is greater than each of the differences in the OPLD values defined in the previous cards. Thus, the simulation would use the next OLPD (and its associated OPLF) before the

current OLPF would be reached.

EXAMPLE

```
OXY FREQ    OPLF    OPLF    OPLF    OPLF    OPLF    OPLF    OPLF    OPLF    OPLF
          365.0   365.0   365.0   365.0   365.0   365.0   365.0   365.0   365.0
          365.0   365.0   365.0   365.0   365.0   365.0   365.0   365.0   365.0
          365.0   365.0   365.0   365.0   365.0   365.0   365.0   365.0   365.0
          365.0   365.0   365.0   365.0   365.0   365.0   365.0   365.0   365.0
          365.0   365.0   365.0   365.0   365.0   365.0
```

Mass Balance Output Control (MASS BAL)

Field	Name	Value	Description
1	MBLC	Character	Specifies if output is written to mass balance file
2	NMBL	Integer	Number of mass balance intervals

This card specifies if mass balances are computed and the number of intervals in which the frequency of the output varies. Mass balances are averaged in a manner similar to the Average Plot file.

EXAMPLE

```
MASS BAL    MBLC    NMBL
             OFF       1
```

Mass Balance Date (MBL DAY)

Field	Name	Value	Description
1-9	MBLD	Real	Date of mass balance interval (Julian day)

This card specifies the intervals at which the mass balance output varies. If there are more intervals than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
MBL DAY     MBLD    MBLD    MBLD    MBLD    MBLD    MBLD    MBLD    MBLD    MBLD
             0.0
```

Mass Balance Frequency (MBL FREQ)

Field	Name	Value	Description
1-9	MBLF	Real	Mass balance output frequency (Julian day)

This card specifies the frequency at which mass balance information is output. If there are more values than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
MBL FREQ    MBLF    MBLF    MBLF    MBLF    MBLF    MBLF    MBLF    MBLF    MBLF
            30.4
```

Diagnostics Output Control (DIAGNSTCS)

Field	Name	Value	Description
1	DIAC	Character	Specifies if output is written to diagnostic file
2	NDIA	Integer	Number of diagnostic intervals

This card specifies if information is output to the diagnostics file and the number of intervals in which the frequency of the output varies.

EXAMPLE

```
DIAGNSTCS   DIAC    NDIA
              ON       1
```

Diagnostics Date (DIA DAY)

Field	Name	Value	Description
1-9	DIAD	Real	Date of diagnostics interval (Julian day)

This card specifies the intervals at which the diagnostics output varies. If there are more intervals than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
DIA DAY     DIAD    DIAD    DIAD    DIAD    DIAD    DIAD    DIAD    DIAD    DIAD
              0.
```

Diagnostic Frequency (DIA FREQ)

Field	Name	Value	Description
1-9	DIAF	Real	Diagnostics output frequency (Julian day)

This card specifies the frequency at which diagnostics information is output. If there are more values than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
DIA FREQ    DIAF    DIAF    DIAF    DIAF    DIAF    DIAF    DIAF    DIAF    DIAF
            1.00
```

Restart Output (RESTART)

Field	Name	Value	Description
1	RSOC	Character	Specifies if output is written to restart file
2	NRSO	Integer	Number of restart output dates
3	RSIC	Character	Specifies if present simulation is generated from a restart file

NOTE: RSIC is read, thus its inclusion is necessary in the Control File, but is a relic variable and is not used in this application.

EXAMPLE

```
RESTART     RSOC    NRSO    RSIC
             OFF       1     OFF
```

Restart Date (RST DAY)

Field	Name	Value	Description
1-9	RSOD	Real	Date of restart output (Julian day)

This card specifies the days at which restart information is output. If there are more restarts than can be specified on one line, then they are continued on the next line.

EXAMPLE

```
RST DAY      RSOD     RSOD     RSOD     RSOD     RSOD     RSOD     RSOD     RSOD     RSOD
           364.0
```

Hydrodynamic Model (HYD MODEL)

Field	Name	Value	Description
1	HYDC	Character	Specifies the type of hydrodynamic model input
2	PREVAPC	Character	Specifies if precipitation and evaporation are considered

This card specifies the nature of hydrodynamic inputs to the water quality model. There are three options for HYDC: "BINARY", "ASCII", and "DEPTH_AV". The BINARY option is usually specified for large files generated by a hydrodynamic model, e.g. CH3D-WES. The ASCII option is usually specified for smaller files which are created independent of a hydrodynamic model. The DEPTH_AV option indicates a two-dimensional (longitudinal-lateral) implementation of the water-quality model with binary input format. PREVAPC specifies if the hydrodynamic model simulated precipitation and evaporation, in which case, hydrodynamic model surface volumes will be used in the water quality model. Otherwise the surface volumes will be calculated internally in the water quality model.

EXAMPLE

```
HYD MODEL    HYDC PREVAPC
           BINARY      ON
```

Hydrodynamic Solution (HYD SOLTN)

Field	Name	Value	Description
1	SLC	Character	Specifies the type of transport solution
2	CONSC	Character	Specifies the type of conservation ` used
3	TH	Real	Crank-Nicholson weighting factor
4	MINSTEP	Real	Specifies Minimum Timestep (seconds)

This card allows the user to specify the type of longitudinal transport scheme that the water quality model uses, how mass is conserved, and the amount of implicit/explicit weighting used in vertical transport. The options for the longitudinal transport scheme are "UPWIND" and "QUICKEST". The upwind option is numerically diffusive which can cause problems during calibration. The QUICKEST option reduces numerical diffusion but can cause overshoots and undershoots in regions of sharp gradients. The model has the capability to use different hydrodynamic files over the period of a simulation. If the hydrodynamic files are disjointed (not continuous in time), the total volume of the system can change when a new hydrodynamic file is used. The abrupt change in volume may cause mass-balance errors in the water-quality model. The user can specify if either mass ("MASS") or concentration ("CONC") is conserved when hydrodynamic files are spanned. If “MASS” is chosen the model will conserve mass but may present concentration discontinuity. If “CONC” is chosen the model will maintain concentrations but may not conserve mass. Theta ("TH") specifies the amount of explicit /implicit time weighting in the vertical transport scheme. A value of zero is fully explicit and a value of one is fully implicit.

EXAMPLE

```
HYD SOLTN    SLC   CONSC      TH MINSTEP
 QUICKEST    MASS    0.75     5.0
```

Miscellaneous Controls (CONTROLS)

Field	Name	Value	Description
1	SEDC	Character	Turns on/off predictive sediment submodel
2	AUTOC	Character	Turns on/off autostepping
3	VBC	Character	Turns on/off volume balance calculations
4	BFOC	Character	Turns on/off output of benthic model parameters and fluxes to designated output file
5	STLC	Character	Turns on/off particle settling
6	ICIC	Character	Specifies format of initial conditions
7	ICOC	Character	Specifies if initial conditions are created for use in a subsequent model run
8	SAVMC	Character	Turns on/off predictive Submerged Aquatic Vegetation submodel

The first five fields must be specified as " ON" or "OFF". The sixth field may be "UNIFORM", "VARIED", OR "BINARY". Descriptions of these options are

provided in the description of the Initial Conditions File. The last two fields must be specified as " ON", or "OFF".

EXAMPLE

```
CONTROLS     SEDC    AUTOC      VBC     BFOC     STLC     ICIC     ICOC    SAVMC
               ON       ON       ON      OFF       ON   BINARY       ON      OFF
```

Benthos Submodel Controls (CONTROLS)

Field	Name	Value	Description
1	SUSFDC	Character	Turns on/off suspension feeders
2	DEPFDC	Character	Turns on/off deposit feeders
3	LOXC	Character	Turns on/off logistic mortality function in benthos submodel

These three fields must be specified as " ON" or "OFF". If SUSFDC and DEPFDC are both “OFF” the value of LOXC is inconsequential since the benthos are both “OFF”.

EXAMPLE

```
CONTROLS  SUSFDC  DEPFDC     LOXC
            OFF     OFF       ON
```

Dead Sea Case (DEAD SEA)

Field	Name	Value	Description
1	FLC	Character	Turns on/off hydrodynamic flows
2	XYDFC	Character	Turns on/off horizontal diffusion
3	ZDFC	Character	Turns on/off vertical diffusion

This card allows the user to turn off any or all transport processes in the model. All fields must be specified as " ON" or "OFF".

EXAMPLE

```
DEAD SEA      FLC    XYDFC     ZDFC
               ON       ON       ON
```

Horizontal Diffusion (HDIFF)

Field	Name	Value	Description
1	XYDF	Real	Value for horizontal diffusion (m^2 s^{-1})
2	ZDFMUL	Real	Multiplier for vertical diffusion
3	ZDFMAX	Real	Maximum vertical diffusion (m^2 s^{-1})

The first application of the water-quality model was in a system with negligible horizontal dispersion. To minimize the size of the hydrodynamic file, dispersion was specified once in the control file rather than written out by the hydrodynamic model at every cell interface, at every time step. This feature is still in place when the BINARY or DEPTH_AV hydrodynamic options are employed. Spatially-variable dispersion is a feature of the model code but the user must perform revisions to read dispersion in binary format. When the ASCII option is employed, spatially- and temporally-varying horizontal dispersion is specified in the hydrodynamic file and the field on this card is ignored.

In the first application of the model, sensitivity runs were performed with varying vertical diffusion. To avoid running the hydrodynamic model repeatedly, a vertical diffusion multiplier was installed in the water-quality model. For similar reasons, specification of maximum vertical diffusion was allowed.

EXAMPLE

```
HDIFF       XYDF  ZDFMUL  ZDFMAX
             2.0    1.00     0.1
```

Constituent Input (CST INPUT)

Field	Name	Value	Description
1	BCC	Character	Turns on/off boundary conditions
2	S1C	Character	Turns on/off first external load file
3	S2C	Character	Turns on/off second external load file
4	S3C	Character	Turns on/off third external load file
5	MDC	Character	Turns on/off modifications to initial concentrations
6	BFC	Character	Turns on/off specified benthic fluxes
7	ATMC	Character	Turns on/off atmospheric inputs
8	SAVLC	Character	Turns on/off submerged aquatic plant inputs

This card allows the user to selectively turn on/off constituent inputs. All fields must be specified as " ON" or "OFF".

EXAMPLE

```
CST INPUT     BCC      S1C      S2C      S3C      MDC      BFC     ATMC    SAVLC
               ON       ON       ON      OFF      OFF      OFF       ON      OFF
```

Nutrient Reductions (NUTR RED)

Field	Name	Value	Description
1	REDS1C	Real	Modifies S1 carbon inputs
2	REDS1N	Real	Modifies S1 nitrogen inputs
3	REDS1P	Real	Modifies S1 phosphorus inputs
4	REDS2C	Real	Modifies S2 carbon inputs
5	REDS2N	Real	Modifies S2 nitrogen inputs
6	REDS2P	Real	Modifies S2 phosphorus inputs
7	REDS3C	Real	Modifies S3 carbon inputs
8	REDS3N	Real	Modifies S3 nitrogen inputs
9	REDS3P	Real	Modifies S3 phosphorus inputs

This card allows the user to selectively modify nutrient loads. Values in the input files are multiplied by the fraction specified on this card. Specification of zero eliminates input values. Specification of unity leaves input values as in the original files. This feature is useful in preliminary investigations of nutrient reduction strategies.

EXAMPLE

```
LOAD RED  REDS1C  REDS1N  REDS1P  REDS2C  REDS2N  REDS2P  REDS3C  REDS3N  REDS3P
            1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
```

Boundary Condition Reductions (BNDC RED)

Field	Name	Value	Description
1	REDCBC	Real	Modifies boundary carbon inputs
2	REDCBN	Real	Modifies boundary nitrogen inputs
3	REDCBP	Real	Modifies boundary phosphorus inputs

This card allows the user to selectively modify boundary conditions. Values in the input files are multiplied by the fraction specified on this card. Specification of zero eliminates input values. Specification of unity leaves input values as in the original files. This feature is useful in preliminary investigations of nutrient

reduction strategies.

EXAMPLE

```
BNDC RED   REDCBC   REDCBN   REDCBP
             1.0      1.0      1.0
```

Boundary Concentrations (BOUNDARY)

Field	Name	Value	Description
1	BNDCC	Character	Specifies how boundary concentrations are handled

This card specifies if input boundary concentrations are updated when the next value is read in from the time-varying data file or if the concentrations are interpolated for each timestep. The inputs are "STEP" or "INTERP". Information regarding these options is found in Chapter 2.

EXAMPLE

```
BOUNDARY    BNDCC
           INTERP
```

Active Constituents (ACT CST)

Field	Name	Value	Description
1-27	ACC	Character	Turns on/off constituent calculations

This card allows the user to turn on/off a state variable for a simulation. Care must be taken when exercising this option because of the interaction of the state variables in the kinetic formulations. Most commonly, this option is used when initially calibrating the water-quality model transport to the hydrodynamic model transport using salinity. This option turns off computations only. All state variables must still be included in load files, boundary conditions, etc. The state variables and their order are

1 Temperature
2 Salinity
3 Suspended Solids
4 Algal Group One
5 Algal Group Two
6 Algal Group Three
7 Zooplankton One
8 Zooplankton Two

9	Dissolved organic carbon
10	Labile particulate carbon
11	Refractory particulate carbon
12	Ammonium
13	Nitrate-nitrite
14	Dissolved organic nitrogen
15	Labile particulate nitrogen
16	Refractory particulate nitrogen
17	Total phosphate
18	Dissolved organic phosphorus
19	Labile particulate phosphorus
20	Refractory particulate phosphorus
21	Chemical oxygen demand
22	Dissolved oxygen
23	Particulate silica
24	Dissolved silica
25	Pathogen
26	Toxic One
27	Toxic Two

EXAMPLE

```
ACT CST      ACC     ACC     ACC     ACC     ACC     ACC     ACC     ACC     ACC
              ON      ON      ON     OFF     OFF      ON     OFF     OFF      ON
              ON      ON      ON      ON      ON      ON      ON      ON      ON
              ON      ON      ON      ON     OFF     OFF      ON     OFF     OFF
```

Number of Files (# FILES)

Field	Name	Value	Description
1	NHYDF	Integer	Number of hydrodynamic files in simulation
2	NTVDF	Integer	Number of time-varying data files in simulation

This card is used to specify the number of time-varying input files, which will be used during the simulation. When the end of a file is reached during the simulation, a new file will be opened. For example, if NTVDF is set to 3, then a new file will be opened each time an end of file is reached until the third file is opened. If an end of file is reached for the last file, the run terminates. Potential time-varying input files are HYD through BFI listed on the next page.

EXAMPLE

```
# FILES     NHYDF   NTVDF
              7       7
```

Input/Output Filenames

Field	Name	Value	Description
1	"File"	Character	Input/output filename

The last cards in the control file specify the names of all input/output files used by the model. This method eliminates the need to know how to link FORTRAN files under a particular operating system. However, it does not preclude linking I/O files. If the user does decide to link files, they must be linked with the names specified by the user on the following cards. Under UNIX and Windows operating systems, full pathnames can be included in the filename specification. The number of hydrodynamic files listed under HYDFN must correspond to the number specified for NHYDF. The same holds true for the other time-varying input files. There must be the exact number specified by NTVDF.

Input File Names

MAPFN	Map file associating model cells with appropriate flow faces.
GEOFN	Geometry file associating cells with their vertical neighbors and associating surface and bottom cells.
ICIFN	Initial conditions file.
AGRFN	Algal growth rate file.
ZOOFN	Zooplankton input file.
SUSFN	Suspension feeders input file.
STLFN	Settling rate file.
MRLFN	Mineralization rate file.
PPTFN	Pathogen or Toxics input file.
EXTFN	Light Extinction input file.
HYDFN	Hydrodynamic input file.
METFN	Meteorological input file.
S1FN	Source One input file.
S2FN	Source Two input file.
S3FN	Source Three input file.
ATMFN	Atmospheric input file.
SAVFN	Submerged Aquatic Vegetation input file.
CBCFN	Boundary Conditions input file.
BFIFN	Benthic Flux input file.

Output File Names

ICOFN	Initial Conditions output file.
SNPFN	ASCII constituent output file.
RSOFN	Restart output file.
PLTFN	Instantaneous Binary constituent output file.
APLFN	Averaged Binary constituent output file.
DIAFN	Diagnostics output file.

TFLFN	Transport Flux output file.
KFLFN	Kinetic Flux output file.
OPLFN	Dissolved Oxygen Volume Days output file.
MBLFN	Mass Balance output file.
ALOFN	Algal output file.
ZFOFN	Zooplankton output file.
BFOFN	Benthic Flux output file.
SVOFN	Submerged Aquatic Vegetation output file.
SUDFN	Suspension Diagnostics output file.
PTOFN	Pathogens and Toxics output file.

Input/Output Filenames (Continued, Non-Time Varying Input files)

EXAMPLE

```
MAP FILE.............................MAPFN.................................
        ../real_inputs/map_LW_11_01_01.inp

GEO FILE.............................GEOFN.................................
        ../real_inputs/geo_LW_11_01_01.inp

ICI FILE.............................ICIFN.................................
        inputs/wqm_ico.jul23

AGR FILE.............................AGRFN.................................
        ../real_inputs/wqm_agr_LW.jul18

ZOO FILE.............................ZOOFN.................................
        wqm_zoo.none

SUS FILE.............................SUSFN.................................
        wqm_sfi.none

STL FILE.............................STLFN.................................
        ../real_inputs/wqm_stl_LW.jul23

MRL FILE.............................MRLFN.................................
        ../inputs/wqm_mrl_LW.jul18

PTT FILE.............................PTTFN.................................
        ../real_inputs/wqm_ptt.june21

EXT FILE.............................EXTFN.................................
        ../real_inputs/wqm_kei_LW.oct22
```

Input/Output Filenames (Continued, Time Varying Hydrodynamic files)

EXAMPLE

```
HYD FILE.............................HYDFN.................................
        /cc2/kim/lake_washington/1995/HYD.INP_0515
        /cc2/kim/lake_washington/1996/HYD.INP_0515
        /cc2/kim/lake_washington/1997/HYD.INP_0515
        /cc2/kim/lake_washington/1995/HYD.INP_0515
        /cc2/kim/lake_washington/1996/HYD.INP_0515
        /cc2/kim/lake_washington/1997/HYD.INP_051
```

Input/Output Filenames (Continued, Time Varying Input files)

```
MET FILE.............................METFN.................................
        ../real_inputs/wqm_met_LW.95
        ../real_inputs/wqm_met_LW.96
        ../real_inputs/wqm_met_LW.97
        ../real_inputs/wqm_met_LW.95
        ../real_inputs/wqm_met_LW.96
        ../real_inputs/wqm_met_LW.97
        ../real_inputs/wqm_met_LW.95

S1  FILE.............................S1FN..................................
        ../real_inputs/wqm_nps_LW.sept16
        ../real_inputs/wqm_nps_LW.sept16
        ../real_inputs/wqm_nps_LW.sept16
        ../real_inputs/wqm_nps_LW.sept16
        ../real_inputs/wqm_nps_LW.9597
        ../real_inputs/wqm_nps_LW.9597
        ../real_inputs/wqm_nps_LW.9597

S2  FILE.............................S2FN..................................
        ../real_inputs/wqm_CSO_LW.9597
        ../real_inputs/wqm_CSO_LW.9597
        ../real_inputs/wqm_CSO_LW.9597
        ../real_inputs/wqm_CSO_LW.9597
        ../real_inputs/wqm_CSO_LW.9597
        ../real_inputs/wqm_CSO_LW.9597
        ../real_inputs/wqm_CSO_LW.9597

S3  FILE.............................S3FN..................................
        wqm_atm.none
        wqm_atm.none5
        wqm_atm.none
        wqm_atm.none
        wqm_atm.none5
        wqm_atm.none
        wqm_atm.none5

ATM FILE.............................ATMFN.................................
        ../real_inputs/wqm_atm.LW
        ../real_inputs/wqm_atm.LW
        ../real_inputs/wqm_atm.LW
        ../real_inputs/wqm_atm.LW
        ../real_inputs/wqm_atm.LW
        ../real_inputs/wqm_atm.LW
        ../real_inputs/wqm_atm.LW

SAV FILE.............................SAVFN.................................
        wqm_sav.none
        wqm_sav.none
        wqm_sav.none
        wqm_sav.none
        wqm_sav.none
        wqm_sav.none
        wqm_sav.none

CBC FILE.............................CBCFN.................................
        ../real_inputs/wqm_cbc_LW.sept16
        ../real_inputs/wqm_cbc_LW.sept16
        ../real_inputs/wqm_cbc_LW.sept16
        ../real_inputs/wqm_cbc_LW.sept16
        ../real_inputs/wqm_cbc_LW.sept16
        ../real_inputs/wqm_cbc_LW.sept16
        ../real_inputs/wqm_cbc_LW.sept16
BFI FILE.............................BFIFN.................................
```

```
../real_inputs/wqm_bfi_LW.jul23
../real_inputs/wqm_bfi_LW.jul23
real_inputs/wqm_bfi_LW.ini
wqm_bfi.none
real_inputs/wqm_bfi_LW.ini
wqm_bfi.none
wqm_bfi.none
```

Input/Output Filenames (Continued, Output files)

EXAMPLE

```
ICO FILE.............................ICOFN.................................
        outputs/wqm_ico.jul23

SNP FILE.............................SNPFN.................................
        wqm_snp.LW_opt

RSO FILE.............................RSOFN.................................
        outputs/wqm_rso.LW_opt

PLT FILE.............................PLTFN.................................
        outputs/wqm_plt.LW_opt

APL FILE.............................APLFN.................................
        outputs/wqm_apl.jul23

DIA FILE.............................DIAFN.................................
        outputs/wqm_dia.jul23

TFL FILE.............................TFLFN.................................
        outputs/wqm_tfl.jul23

KFL FILE.............................KFLFN.................................
        outputs/wqm_kfl.jul23

OPL FILE.............................OPLFN.................................
        outputs/wqm_opl.LW_opt

MBL FILE.............................MBLFN.................................
        outputs/wqm_mbl.LW_opt

ALO FILE.............................ALOFN.................................
        outputs/wqm_alo.LW_opt

ZFO FILE.............................ZFOFN.................................
        outputs/wqm_zfo.LW_opt

BFO FILE.............................BFOFN.................................
        outputs/wqm_bfo.LW_opt

SVO FILE.............................SVOFN.................................
        outputs/wqm_svo.LW_opt

SUD FILE.............................SUDFN.................................
        outputs/wqm_sfo.LW_opt

PTO FILE.............................PTOFN.................................
        outputs/wqm_pto.LW_opt
```

The INCLUDE File

The vast majority of DIMENSION and COMMON statements are coded in a file wqm_com_LW.inc. This file is incorporated into the main program and subroutines through the FORTRAN "INCLUDE" statement. Dimensions of most arrays are specified by the user through PARAMETER statements at the beginning of the INCLUDE file. Specification must take place prior to compilation of the program. For most arrays, dimensions must be greater than or equal to number of corresponding grid elements or model inputs. Variables in PARAMETER statements and their definitions are noted in Table 1.

The INCLUDE file contains the code:

```
REAL*8  V1,       V2,      ELTMS,   ELTMS1
REAL*8  MAXDLTDP, MXDLTDP, NXHYDDP
```

The REAL*8 (DOUBLE PRECISION) statements are required on 32-bit machines including most personal computers and many work stations (e.g. Silicon Graphics Indigo). The REAL*8 statements are not required on 64-bit machines including Cray supercomputers and many newer work stations. For operation on 64-bit machines, the user may remove the "*8" from the REAL statement.

Table 1
Variables in PARAMETER Statements

Variable	Definition
NCP	Number of model state variables. Do not alter the coded value NCP = 27.
NBP	Total number of cells in grid.
NQFP	Total number of flow faces.
NHQP	Number of horizontal flow faces.
NSBP	Number of model cells in surface layer.
NLP	Number of layers in vertical direction.
NS1P	Number of load sources specified in first external load file.
NS2P	Number of load sources specified in second external load file.
NS3P	Number of load sources specified in third external load file.
NBCP	Number of faces at which boundary conditions are specified.
NMP	Number of modifications to uniformly-specified initial conditions.
NDP	Maximum number of days at which plot outputs and similar features are specified.
NSAVP	Number of dominant submerged aquatic vegetation species
NFLP	Maximum number of files for each type of time-varying input data.
NOIP	Maximum number of oxygen-plot intervals.
NSSFP	Number of suspension-feeding species.

The Geometry File

The geometry file has two, alternate formats. The appropriate format depends on the form of hydrodynamic input. When ASCII hydrodynamics are input, the geometry file specifies cell dimensions, cell location in the vertical, and some mapping information. For the ASCII option, cell geometry is invariant. When BINARY hydrodynamics are input, the geometry file specifies minimal mapping information only. The remaining geometric information is input in the hydrodynamics file. BINARY hydrodynamics allow cell geometry to vary due to changes in surface elevation.

ASCII Hydrodynamics

The geometry file described here corresponds to the 30-box grid described in the chapter "Conservation of Mass Equation." The file contains four sections. First, two title cards are available for descriptive purposes but are ignored by the program. Next, cell geometry and location in the vertical are input (5X,3F15.0,F18.0,F12.0,I10). These variables are read in order, starting with cell number 1. The cell number may be listed in the first five columns, but is not read by the program. The depth to the top of the cell is used in the computation of irradiance with depth. The number of the overlying cell is used in computation of particle settling. The next section lists the surface and bottom cell numbers in each cell column (2I10). This information is used in the vertical transport algorithm. Finally, the area of each flow face is provided (13X,F13.0). The sections of geometry, surface and bottom cells, and face area are each preceded by a blank line and a header line.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe geometry file

Two title lines, followed by a blank line, are required to describe the geometry file. These are not read as input but are skipped by a FORMAT statement.

Example

```
Geometry for Zooplankton Model.  Flow face area moved from hydro file.
December 29, 1995.
```

Geometry

Following a header line, cell geometry and location in the vertical are input.

Field	Name	Value	Description
1	Code	Character	Cell number or code (skipped by FORMAT statement)
2	DLL(1)	Real	Cell dimension in direction 1 (as defined in map file, m)
3	DLL(2)	Real	Cell dimension in direction 2 (as defined in map file, m)
4	DLL(3)	Real	Cell dimension in the vertical (m)
5	VH	Real	Cell volume (m^3)
6	ZD	Real	Depth from water surface to top of cell (m)
7	BU	Integer	Cell immediately above this one (specify 0 if this is a surface cell)

Example

B	DLL(1)	DLL(2)	DLL(3)	VH	ZD	BU
1	30000.0	20000.0	5.0	3.0E9	0.0	0
2	30000.0	20000.0	5.0	3.0E9	0.0	0
3	30000.0	20000.0	5.0	3.0E9	0.0	0
4	30000.0	20000.0	5.0	3.0E9	0.0	0
5	30000.0	20000.0	5.0	3.0E9	0.0	0
6	30000.0	20000.0	5.0	3.0E9	0.0	0
7	30000.0	20000.0	5.0	3.0E9	0.0	0
8	30000.0	20000.0	5.0	3.0E9	0.0	0
9	30000.0	20000.0	5.0	3.0E9	0.0	0
10	30000.0	20000.0	5.0	3.0E9	0.0	0
11	30000.0	20000.0	5.0	3.0E9	5.0	1
12	30000.0	20000.0	5.0	3.0E9	5.0	2
13	30000.0	20000.0	5.0	3.0E9	5.0	3
14	30000.0	20000.0	5.0	3.0E9	5.0	4
15	30000.0	20000.0	5.0	3.0E9	5.0	5
16	30000.0	20000.0	5.0	3.0E9	5.0	6
17	30000.0	20000.0	5.0	3.0E9	5.0	7
18	30000.0	20000.0	5.0	3.0E9	5.0	8
19	30000.0	20000.0	5.0	3.0E9	5.0	9
20	30000.0	20000.0	5.0	3.0E9	5.0	10
21	30000.0	20000.0	5.0	3.0E9	10.0	11
22	30000.0	20000.0	5.0	3.0E9	10.0	12
23	30000.0	20000.0	5.0	3.0E9	10.0	13
24	30000.0	20000.0	5.0	3.0E9	10.0	14
25	30000.0	20000.0	5.0	3.0E9	10.0	15
26	30000.0	20000.0	5.0	3.0E9	10.0	16
27	30000.0	20000.0	5.0	3.0E9	10.0	17
28	30000.0	20000.0	5.0	3.0E9	10.0	18
29	30000.0	20000.0	5.0	3.0E9	10.0	19
30	30000.0	20000.0	5.0	3.0E9	10.0	20

Surface and Bottom Boxes

Following a blank line and a header line, the surface and bottom boxes in each column of cells are input. These are understood to be in order starting with surface box number 1 and increasing to the total number of surface boxes.

Field	Name	Value	Description
1	SB	Integer	Surface box
2	BBX	Integer	Bottom box

Example

SB	BBX
1	21
2	22
3	23
4	24
5	25
6	26
7	27
8	28
9	29
10	30

Flow Face Areas

Following a blank line and a header line, the flow face areas are input. These are understood to be in order starting with face number 1 and increasing to the total number of flow faces. The first field can be used to indicate face number but this field is not read in by the program.

Field	Name	Value	Description
1	Code	Integer	Face number or another code (skipped by program)
2	A	Real	Flow face area (m^2)

Example

FACE #	A
1	1.0E5
2	1.0E5
3	1.0E5
4	1.0E5
.	.
.	.
.	.
45	6.0E8
46	6.0E8
47	6.0E8
48	6.0E8
49	6.0E8
50	6.0E8
51	6.0E8

Binary Hydrodynamics

When binary hydrodynamics are employed, most of the geometry information is in the hydrodynamic input file. Only the inputs indicating the location of the cells in the vertical are required. These are input following a conventional two-line title.

Overlying Cell

The cell immediately above each cell is required for computation of settling. These are input in pairs. The program reads these in order starting with cell number 1 and increasing to the number of cells (8X,I8). Note that the first field is not read by the program. The user must exercise caution that the cells pairs are ordered correctly. The overlying cell should be entered as zero for surface cells.

Field	Name	Value	Description
1	BOX	Integer	First cell in cell pair (skipped by program)
2	BUP	Integer	Cell immediately above the first cell

Surface and Bottom Boxes

Following a blank line and a header line, the surface and bottom boxes in each column of cells are input. These are understood to be in order starting with surface box number 1 and increasing to the total number of surface boxes. Note that the format (2I8) differs from the ASCII hydrodynamics.

Field	Name	Value	Description
1	SB	Integer	Surface box
2	BBX	Integer	Bottom box

Example

```
Lake Washington Geometry
 geometry file for ce-qual-ic

     BOX     BUP
       1       0
       2       0
       3       0
       4       0
       5       0
       6       0
       7       0
       8       0
…
     656       1
     657       2
     658       3
     659       4
     660       5
     661       6
     662       7
     663       8
…
   12170   12153
   12171   12163
   12172   12164
   12173   12165
   12174   12169
   12175   12170
   12176   12171
   12177   12172

    sbox    bbox
       1    1284
       2    3048
       3    3049
       4    1892
       5    3599
       6    6432
       7    6831
       8    4134
…
     648    4642
     649    4643
     650    4644
     651    4645
     652    4646
     653    1887
     654    4647
     655    4648
```

The Map File

Introduction

CE-QUAL-ICM employs an unstructured grid. Model cells cannot be referenced on the grid by conventional Cartesian coordinates (e.g. x-y-z). Each cell is located relative to adjacent cells via a "connectivity" or "map file." Because of the nature of "box" models and the transport solution scheme employed in the model, a large amount of information must be specified in the map file.

The map file consists of four portions. First, six title lines are input. Following a blank line and a header line, the linkage between flow faces and cells is specified. Next, following a blank line and a header line, the number of vertical flow faces in each cell column in the grid is listed. Finally, following a blank line and a header line, the vertical face numbers of each vertical flow face are input, by cell column.

In setting up the map file, the user must assign a face number to each flow face. The only restriction in assigning face numbers is that all faces in the X and Y directions must be assigned a number before the vertical faces are assigned a number. Other than this restriction, there is no requirement that face numbers be assigned in any order.

Once the face numbers are assigned to the boxes, the user must specify the direction in which the faces are oriented and the surrounding box numbers. Faces in the X direction are assigned a flow direction of 1, faces in the Y direction are assigned a flow direction of 2, and faces in the Z direction are assigned a flow direction of 3.

The QUICKEST advection scheme uses a three-point interpolation scheme to estimate concentrations at a face. This requires that the solution scheme know the concentration in the two boxes to the left of the face and two boxes to the right of the face (allowing for flow reversals). Thus, for each face, four box numbers are required. The variables ILB, IB, JB, and JRB designate which box is two boxes to the left of the face, which box is immediately left of the face, which box is immediately right of the face, and which box is two boxes right of the face. Positive flow is, by definition, from left to right. If one of these boxes for a given face lies outside the grid, the box number is assigned a value of zero. Faces that exist on an inflow or outflow boundary are defined, but the IB and ILB for positive inflow and the JB and JRB for positive outflow are assigned a value of zero.

The map file format does not change for ASCII or binary hydrodynamics. We present here a complete map file for the thirty-box model described in the chapter "Conservation of Mass Equation" and illustrated in Figure 1. We then present an abbreviated example of the Lake Washington map file.

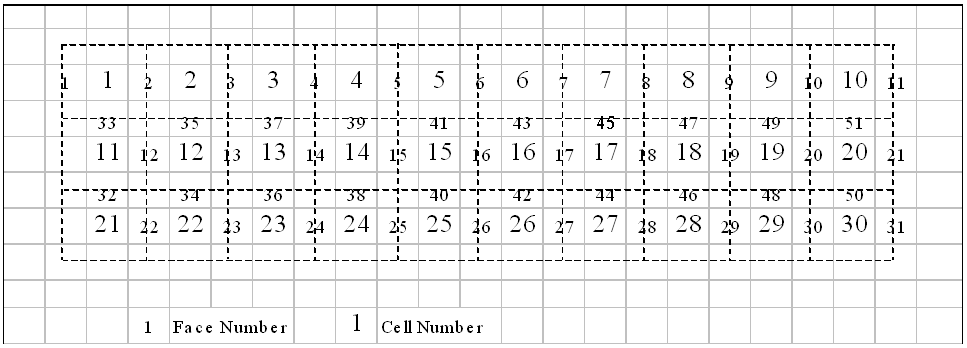

Figure 1. Elevation of thirty-box model

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe geometry file

Six title lines, followed by a blank line, are required to describe the map file. These are not read as input but are skipped by a FORMAT statement.

Example

```
Chesapeake Bay mock up for teaching purposes.
SET UP August 10, 1992
extra title line
extra title line
extra title line
extra title line
```

Flow Faces and Cells

The format for these inputs is (8X,5I8). The first field can be used to identify flow face number but this field is not read by the program. Faces are read in order, starting with face number 1.

Field	Name	Value	Description
1	CODE	Character	Face number or another identifier (skipped by mode READ statement)
2	QD	Integer	Flow direction (1=X, 2=Y, 3=Z)
3	ILB	Integer	I-left box (cell number two cells left of the flow face)
4	IB	Integer	I box (cell number immediately left of the flow face)
5	JB	Integer	J box (cell number immediately right of the flow face)
6	JRB	Integer	J-right box (cell number two cells right of the flow face)

Example

F	QD	IL	IQ	JQ	JR
1	1	0	0	1	2
2	1	0	1	2	3
3	1	1	2	3	4
4	1	2	3	4	5
5	1	3	4	5	6
6	1	4	5	6	7
7	1	5	6	7	8
8	1	6	7	8	9
9	1	7	8	9	10
10	1	8	9	10	0
11	1	9	10	0	0
12	1	0	11	12	13
13	1	11	12	13	14
14	1	12	13	14	15
15	1	13	14	15	16
16	1	14	15	16	17
17	1	15	16	17	18
18	1	16	17	18	19
19	1	17	18	19	20
20	1	18	19	20	0
21	1	19	20	0	0
22	1	0	21	22	23
23	1	21	22	23	24
24	1	22	23	24	25
25	1	23	24	25	26
26	1	24	25	26	27
27	1	25	26	27	28
28	1	26	27	28	29
29	1	27	28	29	30
30	1	28	29	30	0
31	1	29	30	0	0
32	3	0	21	11	1
33	3	21	11	1	0
34	3	0	22	12	2
35	3	22	12	2	0
36	3	0	23	13	3
37	3	23	13	3	0
38	3	0	24	14	4
39	3	24	14	4	0
40	3	0	25	15	5
41	3	25	15	5	0
42	3	0	26	16	6
43	3	26	16	6	0
44	3	0	27	17	7
45	3	27	17	7	0
46	3	0	28	18	8
47	3	28	18	8	0
48	3	0	29	19	9
49	3	29	19	9	0
50	3	0	30	20	10
51	3	30	20	10	0

Number of Vertical Faces

The format for these inputs is (11X,8I8). The number of vertical faces in each column of cells is input. This input is required even for depth-integrated model operation. Columns are read in order starting with surface box number 1 and increasing up to the number of surface boxes. The first field can be used as an identifier but this field is not read by the program.

Field	Name	Value	Description
1	CODE	Character	Cell number or another identifier (skipped by READ statement)
2-9	NVF	Integer	Number of vertical faces

Example

```
 COLUMNS      NVF      NVF      NVF      NVF      NVF      NVF      NVF      NVF
     1-8        2        2        2        2        2        2        2        2
    2-10        2        2
```

Vertical Face Numbers

The format for these inputs is (8X,9I8). The face number of each face in each cell column is input. These are ordered from bottom to top. Each column is read individually so face numbers should not be listed continuously from cell to cell in a single line of input. The first field can be used as an identifier (e.g. surface or bottom cell number) but this field is not read by the program. Columns are read in order starting with surface box number 1 and increasing up to the number of surface boxes. The number of vertical faces listed in each column should agree with the previously specified NVF.

Field	Name	Value	Description
1	CODE	Character	Cell number or another identifier (skipped by READ statement)
2-10	VFN	Integer	Vertical face number, specified from bottom to top of cell column

Example

```
  BBX      VFN      VFN      VFN      VFN      VFN      VFN      VFN      VFN      VFN
   21       32       33
   22       34       35
   23       36       37
   24       38       39
   25       40       41
   26       42       43
   27       44       45
   28       46       47
   29       48       49
   30       50       51
```

Lake Washington Map File

A truncated example of the Lake Washington map file is presented below. This file contains auxiliary information, used to locate cells, that is not read by the program. The user has elected to use blank space, skipped by the read statements, to list grid dimensions, CH3D I-J coordinates, and layer.

Example

```
1 to 1 grid map file for ce-qual-ic
line 3
line 4

  NHQTF     NQF   NSHQF
  21347   32869    1177
      f   qd(f)   il(f)   iq(f)   jq(f)   jr(f)      kp      kf      kl   layer
      1       1       0       1       2       3       2       1       1      41
      2       1       1       2       3       4       3       1       1      41
      3       1       2       3       4       0       4       1       1      41
      4       1       0       5       6       7       2       2       2      41
      5       1       5       6       7       8       3       2       2      41
      6       1       6       7       8       0       4       2       2      41
      7       1       0       9      10      11       2       3       3      41
      8       1       9      10      11      12       3       3       3      41
      9       1      10      11      12       0       4       3       3      41
     10       1       0      13      14      15       2       4       4      41
      .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .
  32865       3    4131    3598    3047    2479       6      22      22      36      37
  32866       3    3598    3047    2479    1889       5      22      22      37      38
  32867       3    3047    2479    1889    1283       4      22      22      38      39
  32868       3    2479    1889    1283     655       3      22      22      39      40
  32869       3    1889    1283     655       0       2      22      22      40      41

 COLUMN         NVF     NVF     NVF     NVF     NVF     NVF     NVF     NVF
   1-    8        2       5       5       3       6      12      13       7
   9-   16        8      16      15       8       9      17      16      10
  17-   24        5       3       0       3       7       6       6       6
  25-   32        3       1       1       1       0       9      18      17
  33-   40       15      12       6       2       7      12      11      10
  41-   48        9       7       4       3       4       3      10      18
  49-   56       18      17      13      10       9      11      11      10
      .         .       .       .       .       .       .       .       .
      .         .       .       .       .       .       .       .       .
      .         .       .       .       .       .       .       .       .
 617-  624        5       2       1       0       0       7       4       7
 625-  632        7       1       7       1       1       7       1       7
 633-  640        7       2       7       7       7       7       7       7
 641-  648        7       7       7       7       7       7       7       7
 649-  656        7       7       7       7       2       7       7

    BBX     VFN     VFN     VFN     VFN     VFN     VFN     VFN     VFN     VFN
   1284   21348   21349
   3048   21350   21351   21352   21353   21354
   3049   21355   21356   21357   21358   21359
   1892   21360   21361   21362
   3599   21363   21364   21365   21366   21367   21368
   6432   21369   21370   21371   21372   21373   21374   21375   21376   21377
          21378   21379   21380
   6831   21381   21382   21383   21384   21385   21386   21387   21388   21389
          21390   21391   21392   21393
    .       .       .       .       .       .       .       .       .       .
    .       .       .       .       .       .       .       .       .       .
    .       .       .       .       .       .       .       .       .       .
   4644   32833   32834   32835   32836   32837   32838   32839
   4645   32840   32841   32842   32843   32844   32845   32846
   4646   32847   32848   32849   32850   32851   32852   32853
```

```
1887   32854   32855
4647   32856   32857   32858   32859   32860   32861   32862
4648   32863   32864   32865   32866   32867   32868   32869
```

The Boundary Conditions File

This file specifies boundary concentrations for all constituents at each boundary face. The file consists of three portions. The first three lines contain header information skipped over by a FORMAT statement. Next, the number of flow faces that are open boundaries is specified. Then the boundary concentrations are input.

The number specified for boundary faces must agree with the number of boundary faces in the map file. These are indicated by pairs of zeroes for the ILB (I left box) and IB (I box) or for JB (J box) and JRB (J right box). The boundary concentrations are entered in the order in which they are encountered within the model code. This is the same order in which the zero pairs occur in the map file. When ICM is coupled to CH3D, the faces are ordered along one CH3D axis, then along the other axis, for each level from surface to bottom. This convention can be awkward. Usually, a preprocessor is employed to translate between convenient boundary specification (e.g. by location or source) and the model format. The number of boundary faces and boundary concentrations must be specified for each of the 27 model constituents even when all constituents are not activated.

Our convention is to specify loads of carbon, nitrogen, phosphorus, bacteria, and solids at river inflows. In this case, boundary concentrations are specified as zero so that loads are not input twice. Concentrations of all substances are conventionally specified at open boundaries such as the junction between an estuary and the ocean. Our convention is not a rule, however. The user may specify pollutant concentrations at inflows, if desired.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe boundary conditions file

Two title lines, followed by a blank line, are required to describe the boundary conditions file. These are not read as input but are skipped by a FORMAT statement.

Example

```
BOUNDARY CONDITIONS FOR LAKE WASHINGTON.  Sept 16, 2002
Use observed ratio Org_C:Org_N, observed split DOC:TOC
```

Number of Boundary Conditions

Following a header line, the number of boundary conditions must be input for each of the 27 model state variables (//(8X,9I8)). This number should be the same for each variable.

Example

```
     NBC      NBC      NBC      NBC      NBC      NBC      NBC      NBC      NBC
      38       38       38       38       38       38       38       38       38
      38       38       38       38       38       38       38       38       38
      38       38       38       38       38       38       38       38       38
```

Boundary Concentrations

A blank line and a header line begin the specification of boundary concentrations. Concentrations can be updated at arbitrary intervals and must be specified at least twice. The first time is at day zero. If the user wishes to maintain the initial boundary conditions throughout the run, the second specification should be on a Julian day greater than the duration of the model run. If the final specification is on a Julian day less than the run duration, the model code will attempt to open a succeeding boundary conditions file.

The first line of concentrations for each variable includes the Julian day on which the boundary condition applies. This day should be the same for each grouping of 27 variables. For convenience, a brief identification code can be placed in the first 8 columns. This field is skipped by the model READ statement, however (8X,9F8.0,:/(:16X,8F8.0)).

Field	Name	Value	Description
1	Code	Character	A variable abbreviation or code (skipped by FORMAT statement)
2	JDAY	Real	Julian day for update of boundary conditions
3 – 10	CBNX	Real	Concentration boundary condition

Example

```
            JDAY    BCOND    BCOND    BCOND    BCOND    BCOND    BCOND    BCOND    BCOND
TEMP        0.00    5.730    5.730    5.730    5.730    5.730    5.730    5.730    5.730
                    5.730    5.730    7.440    5.730    5.730    5.730    5.730    5.730
                    5.730    5.730    7.440    5.730    5.730    5.730    7.440    5.730
                    5.730    5.730    7.440    5.730    5.730    5.730    7.440    5.730
                    5.730    5.730    7.440    5.730    7.440    7.440
SALT        0.00    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
                    0.000    0.000    1.000    0.000    0.000    0.000    0.000    0.000
                    0.000    0.000    1.000    0.000    0.000    0.000    1.000    0.000
                    0.000    0.000    1.000    0.000    0.000    0.000    1.000    0.000
                    0.000    0.000    1.000    0.000    1.000    1.000
ISS         0.00    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
                    0.000    0.000    3.100    0.000    0.000    0.000    0.000    0.000
                    0.000    0.000    3.100    0.000    0.000    0.000    3.100    0.000
                    0.000    0.000    3.100    0.000    0.000    0.000    3.100    0.000
                    0.000    0.000    3.100    0.000    3.100    3.100
ALG 1       0.00    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
                    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
                    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
```

		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000		
ALG 2	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000		
ALG 3	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.095	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.095	0.000	0.000	0.000	0.095	0.000
		0.000	0.000	0.095	0.000	0.000	0.000	0.095	0.000
		0.000	0.000	0.095	0.000	0.095	0.095		
ZOO1	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000		
ZOO2	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000	0.000	0.000		
DOC	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	1.870	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	1.870	0.000	0.000	0.000	1.870	0.000
		0.000	0.000	1.870	0.000	0.000	0.000	1.870	0.000
		0.000	0.000	1.870	0.000	1.870	1.870		
LPOC	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.165	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.165	0.000	0.000	0.000	0.165	0.000
		0.000	0.000	0.165	0.000	0.000	0.000	0.165	0.000
		0.000	0.000	0.165	0.000	0.165	0.165		
RPOC	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.165	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.165	0.000	0.000	0.000	0.165	0.000
		0.000	0.000	0.165	0.000	0.000	0.000	0.165	0.000
		0.000	0.000	0.165	0.000	0.165	0.165		
NH4	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.030	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.030	0.000	0.000	0.000	0.030	0.000
		0.000	0.000	0.030	0.000	0.000	0.000	0.030	0.000
		0.000	0.000	0.030	0.000	0.030	0.030		
NO3	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.250	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.250	0.000	0.000	0.000	0.250	0.000
		0.000	0.000	0.250	0.000	0.000	0.000	0.250	0.000
		0.000	0.000	0.250	0.000	0.250	0.250		
DON	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.093	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.093	0.000	0.000	0.000	0.093	0.000
		0.000	0.000	0.093	0.000	0.000	0.000	0.093	0.000
		0.000	0.000	0.093	0.000	0.093	0.093		
LPON	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.008	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.008	0.000	0.000	0.000	0.008	0.000
		0.000	0.000	0.008	0.000	0.000	0.000	0.008	0.000
		0.000	0.000	0.008	0.000	0.008	0.008		
RPON	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.008	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.008	0.000	0.000	0.000	0.008	0.000
		0.000	0.000	0.008	0.000	0.000	0.000	0.008	0.000
		0.000	0.000	0.008	0.000	0.008	0.008		
PO4	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.012	0.000	0.000	0.000	0.000	0.000
		0.000	0.000	0.012	0.000	0.000	0.000	0.012	0.000
		0.000	0.000	0.012	0.000	0.000	0.000	0.012	0.000
		0.000	0.000	0.012	0.000	0.012	0.012		

```
DOP         0.00   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.003   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.003   0.000   0.000   0.000   0.003   0.000
                   0.000   0.000   0.003   0.000   0.000   0.000   0.003   0.000
                   0.000   0.000   0.003   0.000   0.003   0.003
LPOP        0.00   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.005   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.005   0.000   0.000   0.000   0.005   0.000
                   0.000   0.000   0.005   0.000   0.000   0.000   0.005   0.000
                   0.000   0.000   0.005   0.000   0.005   0.005
RPOP        0.00   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.005   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.005   0.000   0.000   0.000   0.005   0.000
                   0.000   0.000   0.005   0.000   0.000   0.000   0.005   0.000
                   0.000   0.000   0.005   0.000   0.005   0.005
COD         0.00   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000
DO          0.00  10.840  10.840  10.840  10.840  10.840  10.840  10.840  10.840
                  10.840  10.840  10.490  10.840  10.840  10.840  10.840  10.840
                  10.840  10.840  10.490  10.840  10.840  10.840  10.490  10.840
                  10.840  10.840  10.490  10.840  10.840  10.840  10.490  10.840
                  10.840  10.840  10.490  10.840  10.490  10.490
PSIL        0.00   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000
DSIL        0.00   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000
PATH        0.00.000E+00.000E+00.000E+00.000E+00.000E+00.000E+00.000E+00.000E+00
               .000E+00.000E+00.107E+07.000E+00.000E+00.000E+00.000E+00.000E+00
               .000E+00.000E+00.107E+07.000E+00.000E+00.000E+00.107E+07.000E+00
               .000E+00.000E+00.107E+07.000E+00.000E+00.000E+00.107E+07.000E+00
               .000E+00.000E+00.107E+07.000E+00.107E+07.107E+07
TOX1        0.00   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000
TOX2        0.00   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
                   0.000   0.000   0.000   0.000   0.000   0.000
```

External Loads Files

Three files are available for the input of external loads. The format of the files is identical. Provision of three files allows separation of loads by source e.g. point-source and nonpoint-source. Three files also allow updates of loads at different time intervals. One file can list loads at daily intervals while the others lists loads at monthly intervals.

The first two lines in each External Loads file are reserved for identification. The remainder of each file lists the number of loads for each constituent, the cell location for each load, and the loading rate for each cell. Multiple inputs into single cells are allowed. Once specified, loads are held constant until updated. Loads may be updated at arbitrary intervals. The total number of loads and their location cannot be altered.

Number of Loads (NPSLN)

Field	Name	Value	Description
1-27	NPSLN	Integer	Number of external loads for each constituent

This input is required only once at the beginning of the file. The number of loads must be specified for each of 27 state variables, even though not all are active. The format is (8X,9I8). A blank line and a header line precede this input.

EXAMPLE

```
   NPSLN    NPSLN    NPSLN    NPSLN    NPSLN    NPSLN    NPSLN    NPSLN    NPSLN
       0        0       41        0        0        0        0        0       41
      41       41       41       41       41       41       41       41       41
      41       41        0        0        0        0       41        0        0
```

Location of Loads (NPSLB)

Field	Name	Value	Description
1-9	NPSLB	Integer	Cell receiving external load

At least one specification is required for each of the 27 state variables, even though not all are active. The number of cells receiving loads should agree with the variable NPSLN. The format is (8X,9I8). A blank line and a header line precede the specification for each variable. The first 8 columns are not read in and may be used as a code to identify state variables. Variables are read in the order of active constituents:

1 Temperature
2 Salinity
3 Suspended Solids
4 Algal Group One
5 Algal Group Two
6 Algal Group Three
7 Zooplankton One
8 Zooplankton Two
9 Dissolved organic carbon
10 Labile particulate carbon
11 Refractory particulate carbon
12 Ammonium
13 Nitrate-nitrite
14 Dissolved organic nitrogen
15 Labile particulate nitrogen
16 Refractory particulate nitrogen
17 Total phosphate
18 Dissolved organic phosphorus
19 Labile particulate phosphorus
20 Refractory particulate phosphorus
21 Chemical oxygen demand
22 Dissolved oxygen
23 Particulate silica
24 Dissolved silica
25 Pathogen
26 Toxic One
27 Toxic Two

EXAMPLE

```
 ISS   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
         620      86     533     628    1256     629     599     588     549
          86     126     104     216     176      29     135      75     232
         877    1493    2095    2669    3224      19       4      27     681
         189     297     610    1240    1851    2444    3012    3564       2
         657    1285    1890    2480    3048
```

External Load (NPSL)

A blank line and a header line begin the specification of external loads. Loads can be updated at arbitrary intervals and must be specified at least twice. The first time is at day zero. If the user wishes to maintain the initial loads throughout the run, the second specification should be on a Julian day greater than the duration of the model run. If the final specification is on a Julian day less than the run duration, the model code will attempt to open a succeeding external loads file when the last Julian day is exceeded.

The first line of loads for each variable includes the Julian day on which the load applies. This day should be the same for each grouping of 27 variables. For convenience, a brief identification code can be placed in the first 8 columns. This field is skipped by the model READ statement, however (8X,9F8.0,:/(:16X,8F8.0)).

Field	Name	Value	Description
1	Code	Character	A variable abbreviation or code (skipped by FORMAT statement)
2	JDAY	Real	Julian day for update of loads
3 – 10	KG/DAY	Real	Load (kg d^{-1}, except pathogen in 10^6 organisms d^{-1})

Example

```
NPS LOAD     JDAY  KG/DAY  KG/DAY  KG/DAY  KG/DAY  KG/DAY  KG/DAY  KG/DAY  KG/DAY
     ISS      0.    155.     11.     21.     17.     17.      5.     19.     32.
                    45.     30.     60.     37.     23.      5.     40.      2.
                     7.      2.      2.      2.      2.      2.      2.    325.
                     6.     51.     51.    236.  24996.    137.    137.    137.
                   137.    137.    137.  10289.  10289.  10289.  10289.  10289.
                 10289.
```

The following pages illustrate a complete external load file. Loads are initially specified at Julian day 0 and updated at day 30.

```
Point-source example input file
Chesapeake Bay Workshop

# LOADS    NPSLN   NPSLN   NPSLN   NPSLN   NPSLN   NPSLN   NPSLN   NPSLN   NPSLN
               0       0       0       5       0       0       0       0       5
               5       5       5       5       5       5       5       5       5
               5       5       0       0       0       0       0       0       0

    TEMP   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               0

    SALT   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               0

     ISS   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               0

    CYAN   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

    DIAT   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               0

    GREN   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               0

    ZOO1   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               0

    ZOO2   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               0

     DOC   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

    LPOC   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

    RPOC   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

     NH4   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

     NO3   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

     DON   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

    LPON   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

    RPON   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

     PO4   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

     DOP   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

    LPOP   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5

    RPOP   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
               1       2       3       4       5
```

```
      COD   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
                0

       DO   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
                0

     PSIL   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
                0

     DSIL   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
                0

     PATH   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
                0

     TOX1   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
                0

     TOX2   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB   NPSLB
                0

NPS LOAD   JDAY     PSL     PSL     PSL     PSL     PSL     PSL     PSL     PSL
     TEMP     0.      0.
     SALT     0.      0.
      ISS     0.      0.
     CYAN     0.      0.
     DIAT     0.      0.
    GREEN     0.      0.
     ZOO1     0.      0.
     ZOO2     0.      0.
      DOC     0.     10.     10.     10.     10.     10.
     LPOC     0.     18.     10.     10.     10.     10.
     RPOC     0.     10.     10.     10.     10.     10.
      NH4     0.     10.     10.     10.     10.     10.
      NO3     0.     10.     10.     10.     10.     10.
      DON     0.     10.     10.     10.     10.     10.
     LPON     0.     10.     10.     10.     10.     10.
     RPON     0.     10.     10.     10.     10.     10.
      PO4     0.     10.     10.     10.     10.     10.
      DOP     0.     10.     10.     10.     10.     10.
     LPOP     0.     10.     10.     10.     10.     10.
     RPOP     0.     10.     10.     10.     10.     10.
      COD     0.      0.
       DO     0.      0.
     PSIL     0.      0.
     DSIL     0.      0.
     PATH     0.      0.
     TOX1     0.      0.
     TOX2     0.      0.
     TEMP    30.      0.
     SALT    30.      0.
      ISS    30.      0.
     CYAN    30.      0.
     DIAT    30.      0.
    GREEN    30.      0.
     ZOO1    30.      0.
     ZOO2    30.      0.
      DOC    30.     20.     20.     20.     20.     20.
     LPOC    30.     18.     20.     20.     20.     20.
     RPOC    30.     20.     20.     20.     20.     20.
      NH4    30.     20.     20.     20.     20.     20.
      NO3    30.     20.     20.     20.     20.     20.
      DON    30.     20.     20.     20.     20.     20.
     LPON    30.     20.     20.     20.     20.     20.
     RPON    30.     20.     20.     20.     20.     20.
      PO4    30.     20.     20.     20.     20.     20.
      DOP    30.     20.     20.     20.     20.     20.
     LPOP    30.     20.     20.     20.     20.     20.
     RPOP    30.     20.     20.     20.     20.     20.
      COD    30.      0.
       DO    30.      0.
     PSIL    30.      0.
     DSIL    30.      0.
     PATH    30.      0.
     TOX1    30.      0.
     TOX2    30.      0.
```

The Atmospheric Loading File

This file contains the atmospheric loads of nitrogen and phosphorus deposited directly to the water surface. Loads are input in the form of precipitation rate and nutrient concentration within the precipitation. Mass loads to each model cell are computed within the model. Atmospheric loads may be updated on a daily or less frequent basis. Loads input via this file are spatially uniform. For spatially-varying loads, one of the three external loads files can be used.

Loading information is frequently available on a long-term basis, in mg m^{-2} d^{-1}. This was the case for Lake Washington. For loads expressed on this basis, a useful "trick" exists. Specify rainfall as 0.1 cm d^{-1} on day zero. For concentration, specify the loading in mg m^{-2} d^{-1}. (e.g. if loading is 0.25 mg m^{-2} d^{-1}, specify concentration as 0.25 g m^{-3}). The load should be updated on a Julian day greater than the model run duration. That way, the loads will be held constant for the entire run.

The first three cards in the file are title cards for identification or comments. A header card follows. The balance of the file lists precipitation and concentration. The format is (10F8.0).

Field	Name	Value	Description
1	JDAY	Real	Julian day
2	RNFL	Real	Rainfall (cm day^{-1})
3	ATMNH4	Real	Ammonium concentration (gm m^{-3})
4	ATMNO3	Real	Nitrate concentration (gm m^{-3})
5	ATMDON	Real	Dissolved organic nitrogen concentration
6	ATMPO4	Real	Phosphate concentration (gm m^{-3})
7	ATMDOP	Real	Dissolved organic phosphorus concentration (gm m^{-3})

The following cards are an example of an atmospheric loading file.

```
Atmospheric loading file.  AVERAGE VALUES FROM EDMUNDSON &
LEHMAN 1981.  Set up MAY 9, 2002.

    JDAY     RNFL      NH4      NO3      DON      PO4      DOP
     0.0     0.10     0.08     0.50     0.50    0.140    0.130
 10000.      0.10     0.08     0.50     0.50    0.140    0.130
```

The Hydrodynamics File

The Hydrodynamics File has several formats. The appropriate format depends on specification of the variable HYDC in the Control File. If "BINARY" or "DEPTH_AV" are specified, the file is in binary. The "BINARY" option is understood to include multiple cells in the vertical direction. The "DEPTH_AV" specification indicates the grid is only one cell deep. If "ASCII" is specified, the file is in ASCII with no restrictions on dimensionality. Specification of HYDC also determines the contents of the file and forces assumptions about the nature of the hydrodynamics. The BINARY and DEPTH_AV options allow variable surface-cell geometry (to accommodate tidal cycling and other actions) but require uniform, constant horizontal dispersion. The ASCII option requires constant geometry in all cells (including the surface) but accommodates spatially- and temporally-variable dispersion.

The varying features and requirements associated with specification of HYDC were installed during model development to couple with specific hydrodynamic models. No barrier exists, for example, that prevents binary input of variable horizontal dispersion. This input simply was not needed when the model was created. Present features associated with specification of HYDC can be modified through code revisions to the water-quality model. The Lake Washington code is consistent with Z-grid hydrodynamics. Code for sigma grids is available but not distributed with the release version of the CE_QUAL_ICM.

For BINARY and DEPTH_AV hydrodynamics, the first portion of the Hydrodynamics File contains invariant information. Note that this portion of the code is passed over for ASCII hydrodynamics. For ASCII hydrodynamics, the invariant information is entered in the Geometry File. The remainder of the file is devoted to time-variable flows, diffusion, and geometry. The portion of the code that reads the invariant information is given below. Explanation of the variables that appear in the code is provided in Table 1.

```
***** Time-invariant hydrodynamic data

      IF (BINARY_HYDRO) THEN                              !MNOEL 1-25-93
        READ (HYD)  SFA
        READ (HYD) (BL(SB,1),SB=1,NSB)
        READ (HYD) (BL(SB,2),SB=1,NSB)
        READ (HYD) (A(F),F=1,NHQF)
        READ (HYD)  HMBV
        READ (HYD)  HMSBV
      ELSE IF (ASCII_HYDRO) THEN                          !MNOEL 1-25-93
        READ (HYD,1000)
      ELSE IF (DEPTH_AVG_HYDRO) THEN
        READ (HYD)  SFA
        READ (HYD) (A(F),F=1,NHQF)
        READ (HYD) (BL(SB,1),SB=1,NSB)
        READ (HYD) (BL(SB,2),SB=1,NSB)
        READ (HYD)  HMSBV
      ELSE
        WRITE(*,*) 'hydro file specified incorrectly'
        STOP
      END IF
 1000 FORMAT(///)
```

Table 1
Variables Which Define Invariant Hydrodynamics

Variable	Definition	Comments
SFA	Cell surface area (m^2)	Specified for surface cells only. This is an vector with dimension NSBP specified in the INCLUDE File.
BL(SB,1)	Cell length in the x-direction (m)	Specified for surface cells only. BL is a three-dimensional array BL(0:NBP,3). NBP is specified in the INCLUDE File.
BL(SB,2)	Cell length in the y-direction (m)	
NSB	Number of surface cells	Specified in Control File.
A(F)	Flow-face area (m^2)	An vector dimensioned A(0:NQFP). NQFP is specified in the INCLUDE File.
NHQF	Number of horizontal flow faces	Specified in Control File.
NQF	Total number of flow faces	Specified in Control File.
HMBV	Volume of cells below surface layer (m^3)	An array with dimension NSBP. The model assumes that all layers below the surface layer are of uniform thickness. This volume is used to initialize water-quality model volumes.
HMSBV	Volume of cells in the surface layer (m^3)	An array with dimension NSBP. Initial volumes of surface cells may differ from subsurface cells.

Subsequent read operations from the hydrodynamics file are of time-varying input. The coding is complex to allow for end-of-file operations. When an end of file is encountered, the model switches to another file (if one is specified), reinitializes counters, and provides for continuity. A simplified version of the code, that includes only read operations, is shown below.

```
******* Binary time-varying hydrodynamic data

      IF (BINARY_HYDRO) THEN
        READ (HYD,END=10010)          ! Time from hydro model, not used in wqm
               READ (HYD) (A(F),F=1,NSQF)
               READ (HYD) (DIFF(F),F=NHQF+1,NQF)
               READ (HYD)  HMSBV
               READ (HYD) (Q(F),F=1,NHQF)
               READ (HYD) (Q(F),F=NHQF+1,NQF)
               READ (HYD) (QLIT(B),B=1,NB)

******* ASCII time-varying hydrodynamic data

      ELSE IF (ASCII_HYDRO) THEN
          READ (HYD,1000) (Q(F),DIFF(F),F=1,NQF)
          READ (HYD,1005,END=10075) NXDAY
    1000   FORMAT(21X,E10.3,5X,E10.3)

********* depth-averaged hydrodynamics

      ELSE IF (DEPTH_AVG_HYDRO) THEN
        READ (HYD,END=10010)          ! Time from hydro model, not used in wqm
               READ (HYD)  HMSBV
               READ (HYD) (Q(F),F=1,NQF)
               READ (HYD) (A(F),F=1,NSQF)

      END IF
```

Explanation of the variables that appear in the code, and not defined in Table 1, is provided in Table 2.

Table 2
Variables Which Define Time-Variable Hydrodynamics

Variable	Definition	Comments
HYD	Unit number of Hydrodynamics File	Specified as unit 20 in model code.
NSQF	Number of horizontal flow faces in surface layer	Specified in Control File.
DIFF	Diffusion or dispersion coefficient (m^2 sec^{-1}).	An array dimensioned DIFF(0:NQFP). NQFP is specified in the INCLUDE File. For BINARY input, the model reads only vertical diffusion. For ASCII input, the model reads horizontal dispersion and vertical diffusion. For DEPTH_AV input, the model reads no dispersion or diffusion.
Q	Flow	Flow through flow face (m^3 s^{-1})
QLIT	Distributed Flow	Flow not associated with flow face (m^3 s^{-1})

ASCII Hydrodynamics

Input of ASCII hydrodynamics commences with three title lines. These are skipped by the program. A blank line and a header line precede the hydrodynamic inputs. Julian day, flow, and dispersion/diffusion for each flow face are input on individual lines. Although Julian day is input on each line, it is skipped over except for the first flow face. The format is (F8.0,13X,E10.3,5X,E10.3). The blank columns after the Julian day are commonly used to indicate flow face but these are not read in by the program. Flow faces are understood to start with 1 and increase to the number of flow faces.

Flows can be updated at arbitrary intervals and must be specified at least twice. The first time is at day zero. If the user wishes to maintain the initial flows throughout the run, the second specification should be on a Julian day greater than the duration of the model run. If the final specification is on a Julian day less than the run duration, the model code will attempt to open a succeeding hydrodynamics file when the final Julian day is exceeded.

Field	Name	Value	Description
1	JDAY	Real	Julian day for update of hydrodynamics
2	Q	Real	Flow through this face (m^3 s^{-1})
3	DIFF	Real	Diffusion/dispersion at this face (m^2 s^{-1})

Example

A portion of an ASCII hydrodynamic input file for the thirty-cell grid shown in the chapter "Conservation of Mass Equation" is presented below. Hydrodynamics are initially specified at Julian day 0 and updated at day 120.

```
Hydrodynamics for thirty-box zooplankton model.
Flow face areas removed December 29, 1995

    JDAY  FACE #              Q           DIFF
     0.0       1          2000.           10.0
     0.0       2          3000.           10.0
     0.0       3          4000.           10.0
     0.0       4          5000.           10.0
     0.0       5          6000.           10.0
     0.0       6          7000.           10.0
     0.0       7          8000.           10.0
     0.0       8          9000.           10.0
     0.0       9         10000.           10.0
     0.0      10         11000.           10.0
     0.0      11         12000.           10.0
     0.0      12          -500.           10.0
     0.0      13         -1000.           10.0
     0.0      14         -1500.           10.0
     0.0      15         -2000.           10.0
     0.0      16         -2500.           10.0
     0.0      17         -3000.           10.0
     0.0      18         -3500.           10.0
     0.0      19         -4000.           10.0
     0.0      20         -4500.           10.0
     0.0      21         -5000.           10.0
     0.0      22          -500.           10.0
     0.0      23         -1000.           10.0
     0.0      24         -1500.           10.0
     0.0      25         -2000.           10.0
     0.0      26         -2500.           10.0
     0.0      27         -3000.           10.0
     0.0      28         -3500.           10.0
     0.0      29         -4000.           10.0
     0.0      30         -4500.           10.0
     0.0      31         -5000.           10.0
     0.0      32           500.         0.0001
     0.0      33          1000.         0.0001
     0.0      34           500.         0.0001
     0.0      35          1000.         0.0001
     0.0      36           500.         0.0001
     0.0      37          1000.         0.0001
     0.0      38           500.         0.0001
     0.0      39          1000.         0.0001
     0.0      40           500.         0.0001
     0.0      41          1000.         0.0001
     0.0      42           500.         0.0001
     0.0      43          1000.         0.0001
     0.0      44           500.         0.0001
     0.0      45          1000.         0.0001
     0.0      46           500.         0.0001
     0.0      47          1000.         0.0001
```

```
  0.0      48          500.       0.0001
  0.0      49         1000.       0.0001
  0.0      50          500.       0.0001
  0.0      51         1000.       0.0001
120.0       1         2000.           10.0
120.0       2         3000.           10.0
120.0       3         4000.           10.0
120.0       4         5000.           10.0
120.0       5         6000.           10.0
120.0       6         7000.           10.0
120.0       7         8000.           10.0
120.0       8         9000.           10.0
120.0       9        10000.           10.0
120.0      10        11000.           10.0
120.0      11        12000.           10.0
120.0      12         -500.           10.0
120.0      13        -1000.           10.0
120.0      14        -1500.           10.0
120.0      15        -2000.           10.0
120.0      16        -2500.           10.0
120.0      17        -3000.           10.0
120.0      18        -3500.           10.0
120.0      19        -4000.           10.0
120.0      20        -4500.           10.0
120.0      21        -5000.           10.0
120.0      22         -500.           10.0
120.0      23        -1000.           10.0
120.0      24        -1500.           10.0
120.0      25        -2000.           10.0
120.0      26        -2500.           10.0
120.0      27        -3000.           10.0
120.0      28        -3500.           10.0
120.0      29        -4000.           10.0
120.0      30        -4500.           10.0
120.0      31        -5000.           10.0
120.0      32          500.       0.000025
120.0      33         1000.       0.000025
120.0      34          500.       0.000025
120.0      35         1000.       0.000025
120.0      36          500.       0.000025
120.0      37         1000.       0.000025
120.0      38          500.       0.000025
120.0      39         1000.       0.000025
120.0      40          500.       0.000025
120.0      41         1000.       0.000025
120.0      42          500.       0.000025
120.0      43         1000.       0.000025
120.0      44          500.       0.000025
120.0      45         1000.       0.000025
120.0      46          500.       0.000025
120.0      47         1000.       0.000025
120.0      48          500.       0.000025
120.0      49         1000.       0.000025
120.0      50          500.       0.000025
120.0      51         1000.       0.000025
     .           .           .
```

The Initial Conditions File

The Initial Conditions File has three, alternate formats. The appropriate format depends on the initial conditions option specified in the Control File. The options are "UNIFORM", "VARIED", and "BINARY". The UNIFORM option supplies uniform concentrations to each cell in the water column and sediments. (Modifications to the uniform conditions may be specified.) The VARIED option requires specification, in ASCII, of initial concentration in every water column and sediment cell. The BINARY option requires specification, in binary, of initial concentration in every water column and sediment cell. In typical application of the model, uniform conditions are specified for the first model run. After sufficient "spin up" time, model results are output, in ASCII or binary, and employed as initial conditions in subsequent model runs. The format of the ASCII input is identical to the format of output to the Snapshot File so that snapshots at any time interval can be cut from the Snapshot File and used as initial conditions.

The first example provided is for specification of uniform initial conditions. Since the conditions are uniform, this file is appropriate for a grid of any size.

Title

Three lines are available for identifying the file.

EXAMPLE

```
Initial conditions for Lake Washington
Includes modifications for initial sediment conditions
August 15, 1992
```

Initial Concentrations (INIT CONC)

Field	Name	Value	Description
2-10	CIC	Real	Initial concentrations (g m^{-3} except pathogen in mpn m^{-3})

This section specifies initial water-column concentrations for each of the 27 water-column state variables. These must all be specified, even though not all

are active. This section starts with a blank line and a header line. Then concentrations are input using format (8X,9F8.0). The first 8 columns are skipped by the program and may be used for a code or comment.

EXAMPLE

```
INIT CONC    CIC     CIC     CIC     CIC     CIC     CIC     CIC     CIC     CIC
             5.0    25.0     0.0     0.0     0.1     0.1     1.0     1.0     1.0
             1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
             1.0     8.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
```

Initial Sediment Concentrations (INIT SEDC)

Field	Name	Value	Description
1	CTEMP	Real	Initial sediment temperature (^oC)
1	CPOP1	Real	Initial G1 particulate phosphorus concentration (mg m^{-3})
2	CPOP2	Real	Initial G2 particulate phosphorus concentration (mg m^{-3})
3	CPOP3	Real	Initial G3 particulate phosphorus concentration (mg m^{-3})
1	CPON1	Real	Initial G1 particulate nitrogen concentration (mg m^{-3})
2	CPON2	Real	Initial G2 particulate nitrogen concentration (mg m^{-3})
3	CPON3	Real	Initial G3 particulate nitrogen concentration (mg m^{-3})
1	CPOC1	Real	Initial G1 particulate carbon concentration (mg m^{-3})
2	CPOC2	Real	Initial G2 particulate carbon concentration (mg m^{-3})
3	CPOC3	Real	Initial G3 particulate carbon concentration (mg m^{-3})
1	CPOS	Real	Initial particulate biogenic silica concentration (mg m^{-3})
2	PO4T2	Real	Initial phosphate concentration (mg m^{-3})
3	NH4T2	Real	Initial ammonium concentration (mg m^{-3})
4	NO3T2	Real	Initial nitrate concentration (mg m^{-3})
1	HST2	Real	Initial sulfide concentration (mg oxygen equivalents m^{-3})

2	CH4T2	Real	Initial methane concentration in lower layer (mg oxygen equivalents m^{-3})
3	CH41T	Real	Initial methane concentration in upper layer (mg oxygen equivalents m^{-3})
4	SO4T2	Real	Initial sulfate concentration (mg m^{-3})
5	SIT2	Real	Initial dissolved silica concentration (mg m^{-3})
6	BENST	Real	Initial benthic stress
1	BBM	Real	Initial benthic algal biomass (g C m^{-2})

This section specifies the initial sediment concentrations. This section is required only if the predictive sediment model is employed. Each line of input is separated from the preceding line by blank and header lines. The input format is (8X,9F8.0). The first 8 columns are skipped by the program and may be used for a code or comment.

EXAMPLE

```
INIT SEDS  CTEMP
            25.0

           CPOP1   CPOP2   CPOP3
           1000.  10000.  75000.

           CPON1   CPON2   CPON3
          10000. 200000. 750000.

           CPOC1   CPOC2   CPOC3
          50000. 800000.    5.E6

            CPOS   PO4T2   NH4T2   NO3T2
            5.E6  50000.   5000.     50.

            HST2   CH4T2   CH41T   SO4T2    SIT2   BENST
           2000.     0.0     0.0     0.0  75000.     20.

             BBM
      0.0
```

Initial Sediment Toxics Concentrations

Field	Name	Value	Description
1	TOX1S	Real	Initial Toxic 1 concentration ($g\ m^{-3}$)
2	TOX2S	Real	Initial Toxic 2 concentration ($g\ m^{-3}$)

This section specifies the initial toxics concentrations in the sediments. This section is required only if one or more of the toxics state variables is active. This section starts with a blank line and a header line. Then concentrations are input using format (8X,9F8.0). The first 8 columns are skipped by the program and may be used for a code or comment.

EXAMPLE

```
INIT TOXI  TOX1S   TOX2S
           1000.  10000.
```

Initial Deposit and Suspension Feeders

Field	Name	Value	Description
1	DFEED	Real	Initial deposit feeder biomass ($mg\ C\ m^{-2}$)
1	SFEED (1)	Real	Initial Suspension Feeders concentration (1^{st} Species) ($mg\ C\ m^{-2}$)
2	SFEED(2)	Real	Initial Suspension Feeders concentration (2^{nd} Species) ($mg\ C\ m^{-2}$)
N	SFEED(N)	Real	Initial Suspension Feeders concentration (Nth Species) ($mg\ C\ m^{-2}$)

This section specifies the initial Deposit Feeder and Suspension Feeder concentrations. Each of these lines is required if the respective variables are activated. Each line of input is separated from the preceding line by blank and header lines. The input format is (8X,9F8.0). The first 8 columns are skipped by the program and may be used for a code or comment.

EXAMPLE

```
INITDFEED  DFEED
           1000.

INITSFEED SFEED1  SFEED2  SFEED3
          10000.  10000.  10000.
```

Initial Submerged Aquatic Vegetation Densities

Field	Name	Value	Description
1	SH	Real	Initial shoot density (g C m^{-2})
2	EP	Real	Initial epiphyte density (g epiphyte C g^{-1} shoot C)
3	RT	Real	Initial root density (g C m^{-2})

This section specifies the Submerged Aquatic Vegetation densities. This section is required only if the predictive submerged aquatic vegetation model is employed. This section starts with a blank line and a header line. Then densities are input using format (8X,9F8.0). The first 8 columns are skipped by the program and may be used for a code or comment.

EXAMPLE

```
INIT  SAV    SH      EP       RT
           1000.  10000.     1.0
```

Number of Modifications (# MOD)

Field	Name	Value	Description
2-10	NMOD	Integer	Specifies number of cells to modify initial concentrations

This input specifies how many cells will have their initial concentrations modified for each of the 27 water-column state variables. These must all be specified, even though not all are active. This section starts with a blank line and a header line. The number of cells are input using format (8X,9I8). The first 8 columns are skipped by the program and may be used for a code or comment. Typically, modifications are employed to simulate dye injections and in mass-conservation studies.

EXAMPLE

```
# MOD       NMOD     NMOD     NMOD     NMOD     NMOD     NMOD     NMOD     NMOD     NMOD
              3        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
```

Modifications

Input to this group consists of six lines for each water-column state variable. These must all be specified, even though all variables are not active. Following a blank line and a header line, the cell number of the constituent to be modified is input. If there are no modifications to be made, the value for the cell number can be left blank or a zero value may be entered. The number of values entered must correspond to the value given for NMOD previously. Format for these inputs is (//(8X,9I8). The first 8 columns are skipped by the program and may be used for a code or comment. Following another blank and header line, the modified concentrations are input. The number of values entered must correspond to the value given for NMOD previously. Format for these inputs is (//(8X,9F8.0). The first 8 columns are skipped by the program and may be used for a code or comment.

Field	Name	Value	Description
2-10	BMOD	Integer	Cell in which concentration is modified
2-10	CMOD	Real	Modified concentration (g m^{-3} except pathogen in mpn m^{-3})

EXAMPLE

```
T       BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD
          1       5      10

        CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD
        30.0    30.0    30.0
```

Example of Uniform Input File

The following example illustrates the complete initial conditions file when uniform conditions are specified.

```
INITIAL CONDITIONS FOR THIRTY-SEGMENT BAY MOCKUP.
INCLUDES MOD FOR INITIAL SEDIMENT CONDITIONS.  AUGUST 11, 1992

INIT CONC    CIC     CIC     CIC     CIC     CIC     CIC     CIC     CIC     CIC
             5.0    25.0     0.0     0.0     0.1     0.1     1.0     1.0     1.0
             1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
             1.0     8.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0

INIT SEDS  CTEMP
            25.0

           CPOP1   CPOP2   CPOP3
           1000.  10000.  75000.

           CPON1   CPON2   CPON3
          10000. 200000. 750000.

           CPOC1   CPOC2   CPOC3
          50000. 800000.    5.E6

            CPOS   PO4T2   NH4T2   NO3T2
            5.E6  50000.   5000.     50.

            HST2   CH4T2   CH41T   SO4T2    SIT2   BENST
           2000.     0.0     0.0     0.0  75000.     20.

             BBM
             0.0

INIT TOXI  TOX1S   TOX2S
           1000.  10000.

INITDFEED  DFEED
           1000.

INITSFEED SFEED1  SFEED2  SFEED3
          10000.  10000.  10000.

INIT  SAV    SH      EP       RT
           1000.  10000.     1.0

# MOD       NMOD    NMOD    NMOD    NMOD    NMOD    NMOD    NMOD    NMOD    NMOD
               3       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

    T       BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD
               1       5      10

           CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD
           30.0    30.0    30.0

 SALT      BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD


           CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD


  SSI      BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD


           CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD









 ALG1      BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD    BMOD


           CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD    CMOD
```

ALG2	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
ALG3	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
ZOO1	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
ZOO2	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
DOC	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
LPOC	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
RPOC	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
NH4	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
NO3	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
DON	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
LPON	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
RPON	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
PO4	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
DOP	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD

	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
LPOP	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
RPOP	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
COD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
DO	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
SU	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
SA	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
PATH	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
TOX1	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD
TOX2	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD	BMOD
	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD	CMOD

Variable Initial Conditions

Uniform initial conditions were the only option when the model was first developed. Soon, the need to "loop" initial conditions became apparent. This looping is effectively the only way to initialize conditions in the sediments. Consequently, the ability to utilize a portion of the snapshot file from a preceding run as initial conditions was developed. This ability remains in the model as the "VARIABLE" initial conditions option. This feature is little-used and not recommended. For practical operations (more than 10,000 cells) the snapshot file is unwieldy and the formatting is awkward. The "BINARY" option is almost always used to specify variable initial conditions. The use of binary initial conditions is transparent to the user. The binary initial conditions file produced by one run can be used in any succeeding run, provided the number of state variables does not change. Also, living resources such as SAV cannot be activated or de-activated in between the creation and employment of a binary initial conditions file. On occasion, we have the need to create a variable initial conditions file or to use only a portion of a binary file (e.g. loop sediments but not water column). This need arises especially when the water column conditions at the end of a run are substantially different than at the beginning of a run. In that case, we write a pre-processor that will create an appropriate binary initial conditions file.

Water Quality Model Formulation

Introduction

CE-QUAL-ICM was designed to be a flexible, widely-applicable eutrophication model. Initial application was to Chesapeake Bay (Cerco and Cole 1994). Subsequent additional applications included the Delaware Inland Bays (Cerco et al. 1994), Newark Bay (Cerco and Bunch 1997), and the San Juan Bay Estuary (Bunch et al. 2000). Each model application employed a different combination of model features and required addition of system-specific capabilities. This chapter describes general features and site-specific developments of the model as presently applied to the water column of Lake Washington.

Conservation of Mass Equation

The foundation of CE-QUAL-ICM is the solution to the three-dimensional mass-conservation equation for a control volume. Control volumes correspond to cells on the model grid. CE-QUAL-ICM solves, for each volume and for each state variable, the equation:

$$\frac{\delta V_j \bullet C_j}{\delta t} = \sum_{k=1}^{n} Q_k \bullet C_k + \sum_{k=1}^{n} A_k \bullet D_k \bullet \frac{\delta C}{\delta x_k} + \Sigma S_j$$

Equation 1

in which:

V_j = volume of j^{th} control volume (m^3)
C_j = concentration in j^{th} control volume (g m^{-3})
t, x = temporal and spatial coordinates
n = number of flow faces attached to j^{th} control volume
Q_k = volumetric flow across flow face k of j^{th} control volume (m^3 s^{-1})
C_k = concentration in flow across face k (g m^{-3})
A_k = area of flow face k (m^2)
D_k = diffusion coefficient at flow face k (m^2 s^{-1})

S_j = external loads and kinetic sources and sinks in j^{th} control volume (g s^{-1})

Solution of Equation 1 on a digital computer requires discretization of the continuous derivatives and specification of parameter values. The equation is solved using the QUICKEST algorithm (Leonard 1979) in the horizontal plane and a Crank-Nicolson scheme in the vertical direction. Discrete time steps, determined by computational stability requirements, are .15 minutes.

State Variables

As applied to Lake Washington, the CE-QUAL-ICM model incorporates 20 state variables in the water column including physical variables, phytoplankton, multiple forms of carbon, nitrogen, and phosphorus, a pathogen, and two toxicants (Table 1). The pathogen and toxicants were added specifically for the Lake Washington application and are described in a subsequent chapter.

Algae

The coding of CE-QUAL-ICM allows the specification of up to three algal groups. One group is presently activated for Lake Washington.

Zooplankton

The coding of CE-QUAL-ICM allows the specification of two zooplankton groups: microzooplankton and mesozooplankton. These are not presently activated.

Organic Carbon

Three organic carbon state variables are considered: dissolved, labile particulate, and refractory particulate. Labile and refractory distinctions are based upon the time scale of decomposition. Labile organic carbon decomposes on a time scale of days to weeks while refractory organic carbon requires more time. Labile organic carbon decomposes rapidly in the water column or the sediments. Refractory organic carbon decomposes slowly, primarily in the sediments, and may contribute to sediment oxygen demand years after deposition.

Nitrogen

Nitrogen is first divided into available and unavailable fractions. Available refers to employment in algal nutrition. Two available forms are considered: reduced and oxidized nitrogen. For the Lake Washington application, reduced nitrogen consists exclusively of ammonium. Nitrate and nitrite comprise the oxidized nitrogen pool. Both reduced and oxidized nitrogen are utilized to fulfill algal nutrient requirements. The primary reason for distinguishing the two is that ammonium is oxidized by nitrifying bacteria into nitrite and, subsequently, nitrate. This oxidation can be a significant sink of oxygen in the water column and sediments.

Unavailable nitrogen state variables are dissolved organic nitrogen, labile particulate organic nitrogen, and refractory particulate organic nitrogen.

Phosphorus

As with nitrogen, phosphorus is first divided into available and unavailable fractions. Only a single available form, dissolved phosphate, is considered. The model framework allows for exchange of phosphate between dissolved and particulate (sorbed to solids) forms but this option is not implemented in the present application. Three forms of unavailable phosphorus are considered: dissolved organic phosphorus, labile particulate organic phosphorus, and refractory particulate organic phosphorus.

Silica

Silica is included in the complete version of CE-QUAL-ICM but is not activated in the Lake Washington application.

Chemical Oxygen Demand

Chemical oxygen demand is the concentration of reduced substances that are oxidized by abiotic processes. In freshwater, a primary component of chemical oxygen demand is methane released from sediments. Oxidation of methane may remove substantial quantities of dissolved oxygen from the water column.

Dissolved Oxygen

Dissolved oxygen is required for the existence of higher life forms. Oxygen availability determines the distribution of organisms and the flows of energy and nutrients in an ecosystem. Dissolved oxygen is a central component of the water-quality model.

Salinity

Salinity is included in the coding of CE-QUAL-ICM but is not activated in Lake Washington at present

Temperature

Temperature is a primary determinant of the rate of biochemical reactions. Reaction rates increase as a function of temperature although extreme temperatures may result in the mortality of organisms and a decrease in kinetics rates.

Fixed Solids

Fixed solids are the mineral fraction of total suspended solids. Solids are

considered primarily for their role in light attenuation.

The remainder of this chapter is devoted to detailing the kinetics sources and sinks and to reporting parameter values. For notational simplicity, the transport terms are dropped in the reporting of kinetics formulations.

Algae

Algal sources and sinks in the conservation equation include production, metabolism, predation, and settling. These are expressed:

$$\frac{\delta}{\delta t} B = \left(G - BM - Wa \bullet \frac{\delta}{\delta z} \right) B - PR$$

Equation 2

in which:

B = algal biomass, expressed as carbon (g C m^{-3})
G = growth (d^{-1})
BM = basal metabolism (d^{-1})
Wa = algal settling velocity (m d^{-1})
PR = predation (g C m^{-3} d^{-1})
z = vertical coordinate

Production

Production by phytoplankton is determined by the intensity of light, by the availability of nutrients, and by the ambient temperature.

Light

The influence of light on phytoplankton production is represented by a chlorophyll-specific production equation (Jassby and Platt 1976):

$$P^B = P^B m \frac{I}{\sqrt{I^2 + Ik^2}}$$

Equation 3

in which:

P^B = photosynthetic rate (g C g^{-1} Chl d^{-1})
$P^B m$ = maximum photosynthetic rate (g C g^{-1} Chl d^{-1})
I = irradiance (E m^{-2} d^{-1})

Parameter Ik is defined as the irradiance at which the initial slope of the production vs. irradiance relationship (Figure 1) intersects the value of $P^B m$:

$$Ik = \frac{P^B m}{\alpha}$$

Equation 4

in which:

α = initial slope of production vs. irradiance relationship (g C g^{-1} Chl ($E\ m^{-2}$)$^{-1}$)

Chlorophyll-specific production rate is readily converted to carbon specific growth rate, for use in Equation 2, through division by the carbon-to-chlorophyll ratio:

$$G = \frac{P^B}{CChl}$$

Equation 5

in which:

CChl = carbon-to-chlorophyll ratio (g C g^{-1} chlorophyll a)

Nutrients

Carbon, nitrogen, and phosphorus are the primary nutrients required for algal growth. Inorganic carbon is usually available in excess and is not considered in the model. The effects of the remaining nutrients on growth are described by the formulation commonly referred to as "Michaelis-Menton kinetics" (Figure 2):

$$f(N) = \frac{D}{KHd + D}$$

Equation 6

in which:

f(N) = nutrient limitation on algal production ($0 \leq f(N) \leq 1$)
D = concentration of dissolved nutrient (g m^{-3})
KHd = half-saturation constant for nutrient uptake (g m^{-3})

Temperature

Algal production increases as a function of temperature until an optimum temperature or temperature range is reached. Above the optimum, production declines until a temperature lethal to the organisms is attained. Numerous functional representations of temperature effects are available. Inspection of growth versus temperature data indicates a function similar to a Gaussian probability curve (Figure 3) provides a good fit to observations:

$$f(T) = e^{-KTg1 \bullet (T - Topt)^2} \; when \; T \leq Topt$$

$$= e^{-KTg2 \bullet (Topt - T)^2} \; when \; T > Topt$$

Equation 7

in which:

T = temperature (^oC)
Topt = optimal temperature for algal growth (^oC)
KTg1 = effect of temperature below Topt on growth ($^oC^{-2}$)
KTg2 = effect of temperature above Topt on growth ($^oC^{-2}$)

Constructing the Photosynthesis vs. Irradiance Curve

A production versus irradiance relationship is constructed for each model cell at each time step. First, the maximum photosynthetic rate under ambient temperature and nutrient concentrations is determined:

$$P^B m(N,T) = P^B m \bullet f(T) \bullet \frac{D}{KHd + D}$$

Equation 8

in which:

$P^B m(N,T)$ = maximum photosynthetic rate under ambient temperature and nutrient concentrations (g C g^{-1} Chl d^{-1})

The single most limiting nutrient is employed in determining the nutrient limitation.

Next, parameter Ik is derived from Equation 4. Finally, the production vs. irradiance relationship is constructed using $P^B m(N,T)$ and Ik. The resulting production versus irradiance curve exhibits three regions (Figure 4). For I >> Ik, the value of the term $I / (I^2 + Ik^2)^2$ approaches unity and temperature and nutrients are the primary factors that influence production. For I << Ik, production is determined solely by α and irradiance I. In the region where the initial slope of the production versus irradiance curve intercepts the line

indicating production at optimal illumination, I . Ik, production is determined by the combined effects of temperature, nutrients, and light.

Irradiance

Solar radiation at the water surface is input to the model as part of the heat transfer calculations. An empirical conversion is employed to convert between short-wave solar radiation and photosynthetically-active radiation (Einsteins m^{-2} = 0.143 ● watts m^{-2})

Respiration

Two forms of respiration are considered in the model: photo-respiration and basal metabolism. Photo-respiration represents the energy expended by carbon fixation and is a fixed fraction of production. In the event of no production (e.g. at night), photo-respiration is zero. Basal metabolism is a continuous energy expenditure to maintain basic life processes. In the model, metabolism is considered to be an exponentially increasing function of temperature (Figure 5). Total respiration is represented:

$$R = Presp \bullet G + BM \bullet e^{KTb \bullet (T - Tr)}$$

Equation 9

in which:

Presp = photo-respiration ($0 \leq Presp \leq 1$)
BM = metabolic rate at reference temperature Tr (d^{-1})
KTb = effect of temperature on metabolism ($^oC^{-1}$)
Tr = reference temperature for metabolism (^oC)

Predation

The predation term includes the activity of zooplankton, filter-feeding benthos, and other pelagic filter feeders including planktivorous fish. A variety of formulations are available to represent predation. For Lake Washington, a piecewise linear predation term worked well:

$$PR = BPR \bullet B$$

Equation 10

in which:

BPR = base predation rate (d^{-1})

Accounting for Algal Phosphorus

The amount of phosphorus incorporated in algal biomass is quantified through a stoichiometric ratio. Thus, total phosphorus in the model is expressed: in which:

$$TotP = PO_4 + Apc \bullet B + DOP + LPOP + RPOP$$

Equation 11

TotP = total phosphorus (g P m^{-3})
PO_4 = dissolved phosphate (g P m^{-3})
Apc = algal phosphorus-to-carbon ratio (g P g^{-1} C)
DOP = dissolved organic phosphorus (g P m^{-3})
LPP = labile particulate organic phosphorus (g P m^{-3})
RPP = refractory particulate organic phosphorus (g P m^{-3})

Algae take up dissolved phosphate during production and release dissolved phosphate and organic phosphorus through respiration. The fate of phosphorus released by respiration is determined by empirical distribution coefficients (Table 2). The fate of algal phosphorus recycled by predation is determined by a second set of distribution parameters.

Accounting for Algal Nitrogen

Model nitrogen state variables include ammonium, nitrate+nitrite, dissolved organic nitrogen, labile particulate organic nitrogen, and refractory particulate organic nitrogen. The amount of nitrogen incorporated in algal biomass is quantified through a stoichiometric ratio. Thus, total nitrogen in the model is expressed:

$$TotN = NH_4 + NO_{23}$$

$$+ Anc \bullet B + DON + LPON + RPON$$

Equation 12

in which:

TotN = total nitrogen (g N m^{-3})
NH_4 = ammonium (g N m^{-3})
NO_{23} = nitrate+nitrite (g N m^{-3})
Anc = algal nitrogen-to-carbon ratio (g N g^{-1} C)
DON = dissolved organic nitrogen (g N m^{-3})
LPON = labile particulate organic nitrogen (g N m^{-3})

RPON = refractory particulate organic nitrogen (g N m^{-3})

As with phosphorus, the fate of algal nitrogen released by metabolism and predation is represented by distribution coefficients (Table 2).

Algal Nitrogen Preference

Algae take up ammonium and nitrate+nitrite during production and release ammonium and organic nitrogen through respiration. Nitrate+nitrite is internally reduced to ammonium before synthesis into biomass occurs (Parsons et al. 1984). Trace concentrations of ammonium inhibit nitrate reduction so that, in the presence of multiple nitrogenous nutrients, ammonium is utilized first. The "preference" of algae for ammonium is expressed by an empirical function (Thomann and Fitzpatrick 1982):

$$PN = NH_4 \bullet \frac{NO_{23}}{(KHn + NH_4) \bullet (KHn + NO_{23})} + NH_4 \bullet \frac{KHn}{(NH_4 + NO_{23}) \bullet (KHn + NO_{23})}$$

Equation 13

in which

PN = algal preference for ammonium uptake ($0 \leq Pn \leq 1$)
KHn = half saturation concentration for algal nitrogen uptake (g N m^{-3})

The function has two limiting values (Figure 6). When nitrate+nitrite is absent, the preference for ammonium is unity. When ammonium is absent, the preference is zero. In the presence of ammonium and nitrate+nitrite, the preference depends on the abundance of both forms relative to the half-saturation constant for nitrogen uptake. When both ammonium and nitrate+nitrite are abundant, the preference for ammonium approaches unity. When ammonium is scarce but nitrate+nitrite is abundant, the preference decreases in magnitude and a significant fraction of algal nitrogen requirement comes from nitrate+nitrite.

Effect of Algae on Dissolved Oxygen

Algae produce oxygen during photosynthesis and consume oxygen through respiration. The quantity produced depends on the form of nitrogen utilized for growth. More oxygen is produced, per unit of carbon fixed, when nitrate is the algal nitrogen source than when ammonium is the source. Equations describing algal uptake of carbon and nitrogen and production of dissolved oxygen (Morel 1983) are:

$$106\ CO_2 + 16\ NH_4^+ + H_2PO_4^- + 106\ H_2O \text{ --> }$$

$$\text{protoplasm} + 106\ O_2 + 15\ H^+$$

Equation 14

$$106\ CO_2 + 16\ NO_3^- + H_2PO_4^- + 122\ H_2O + 17\ H^+ \text{ --> }$$

$$\text{protoplasm} + 138\ O_2$$

Equation 15

When ammonium is the nitrogen source, one mole oxygen is produced per mole carbon dioxide fixed. When nitrate is the nitrogen source, 1.3 moles oxygen are produced per mole carbon dioxide fixed.

The equation that describes the effect of algae on dissolved oxygen in the model is:

$$\frac{\delta}{\delta t} DO = \left[(1.3 - 0.3 \bullet PN) \bullet P - (1 - FCD) \bullet BM\right] \bullet AOCR \bullet B$$

Equation 16

in which:

FCD = fraction of algal metabolism recycled as dissolved organic carbon ($0 \leq FCD \leq 1$)
AOCR = dissolved oxygen-to-carbon ratio in respiration (2.67 g O_2 g^{-1} C)

The magnitude of AOCR is derived from a simple representation of the respiration process:

$$CH_2O + O_2 = CO_2 + H_2O$$

Equation 17

The quantity (1.3 - 0.3 ● PN) is the photosynthesis ratio and expresses the molar quantity of oxygen produced per mole carbon fixed. The photosynthesis ratio approaches unity as the algal preference for ammonium approaches unity.

Organic Carbon

Organic carbon undergoes innumerable transformations in the water column. The model carbon cycle (Figure 7) consists of the following elements:

Phytoplankton production and excretion
Predation on phytoplankton
Dissolution of particulate carbon
Heterotrophic respiration
Denitrification
Settling

Algal production is the primary carbon source although carbon also enters the system through external loading. Predation on algae by zooplankton and other organisms releases particulate and dissolved organic carbon to the water column. A fraction of the particulate organic carbon undergoes first-order dissolution to dissolved organic carbon. Dissolved organic carbon produced by excretion, by predation, and by dissolution is respired at a first-order rate to inorganic carbon. Particulate organic carbon that does not undergo dissolution settles to the bottom sediments.

Dissolution and Respiration

Organic carbon dissolution and respiration are represented as first-order processes in which the reaction rate is proportional to concentration of the reactant. An exponential function (Figure 5) relates dissolution and respiration to temperature.

In the model, a Monod-like function diminishes respiration as dissolved oxygen approaches zero. As oxygen is depleted from natural systems, oxidation of organic matter is effected by the reduction of alternate oxidants. The sequence in which alternate oxidants are employed is determined by the thermodynamics of oxidation-reduction reactions. The first substance reduced in the absence of oxygen is nitrate. A representation of the denitrification reaction can be obtained by balancing standard half-cell redox reactions (Stumm and Morgan 1981):

$$4\ NO_3^- + 4\ H^+ + 5\ CH_2O \text{ --> } 2\ N_2 + 7\ H_2O + 5\ CO_2$$

Equation 18

Equation 18 describes the stoichiometry of the denitrification reaction. The kinetics of the reaction, as represented in the model, are first-order. The dissolved organic carbon respiration rate, Kdoc, is modified so that significant decay via denitrification occurs only when nitrate is freely available and dissolved oxygen is depleted (Figure 8). A parameter is included so that the anoxic respiration rate is slower than oxic respiration:

$$Denit = \frac{KHodoc}{KHodoc + DO} \bullet \frac{NO_3}{KHndn + NO_3} \bullet AANOX \bullet Kdoc$$

Equation 19

in which:

Denit = denitrification rate of dissolved organic carbon (d^{-1})
Kdoc = first-order dissolved organic carbon respiration rate (d^{-1})
AANOX = ratio of denitrification to oxic carbon respiration rate
($0 \leq AANOX \leq 1$)
KHodoc = half-saturation concentration of dissolved oxygen required for oxic respiration ($g\ O_2\ m^{-3}$)
KHndn = half-saturation concentration of nitrate required for denitrification
($g\ N\ m^{-3}$)

Dissolved Organic Carbon

The complete representation of dissolved organic carbon sources and sinks in the model ecosystem is:

$$\frac{\delta}{\delta t} DOC = FCD \bullet R \bullet B + FCDP \bullet PR + Klpoc \bullet LPOC$$
$$+ Krpoc \bullet RPOC - \frac{DO}{KHodoc + DO} \bullet Kdoc \bullet DOC - DENIT \bullet DOC$$

Equation 20

in which:

DOC = dissolved organic carbon ($g\ m^{-3}$)
LPOC = labile particulate organic carbon ($g\ m^{-3}$)
RPOC = refractory particulate organic carbon ($g\ m^{-3}$)
FCD = fraction of algal respiration released as DOC ($0 < FCD < 1$)
FCDP = fraction of predation on algae released as DOC ($0 < FCDP < 1$)
Klpoc = dissolution rate of LPOC (d^{-1})
Krpoc = dissolution rate of RPOC (d^{-1})
Kdoc = respiration rate of DOC (d^{-1})

Labile Particulate Organic Carbon

The complete representation of labile particulate organic carbon sources and sinks in the model ecosystem is:

$$\frac{\delta}{\delta t} LPOC = FCL \bullet R \bullet B + FCLP \bullet PR - Klpoc \bullet LPOC - Wl \bullet \frac{\delta}{\delta z} LPOC$$

Equation 21

in which:

FCL = fraction of algal respiration released as LPOC ($0 < FCL < 1$)
FCLP = fraction of predation on algae released as LPOC ($0 < FCLP < 1$)
Wl = settling velocity of labile particles (m d^{-1})

Refractory Particulate Organic Carbon

The complete representation of refractory particulate organic carbon sources and sinks in the model ecosystem is:

$$\frac{\delta}{\delta t} RPOC = FCR \bullet R \bullet B + FCRP \bullet PR - Krpoc \bullet RPOC - Wr \bullet \frac{\delta}{\delta z} RPOC$$

Equation 22

in which:

FCR = fraction of algal respiration released as RPOC ($0 < FCR < 1$)
FCRP = fraction of predation on algae released as RPOC ($0 < FCRP < 1$)
Wr = settling velocity of refractory particles (m d^{-1})

Phosphorus

The model phosphorus cycle (Figure 9) includes the following processes:

Algal uptake and excretion
Predation
Hydrolysis of particulate organic phosphorus
Mineralization of dissolved organic phosphorus
Settling and resuspension

External loads provide the ultimate source of phosphorus to the system.

Dissolved phosphate is incorporated by algae during growth and released as phosphate and organic phosphorus through respiration and predation. Dissolved organic phosphorus is mineralized to phosphate. A portion of the particulate organic phosphorus hydrolyzes to dissolved organic phosphorus. The balance settles to the sediments. Within the sediments, particulate phosphorus is mineralized and recycled to the water column as dissolved phosphate.

Hydrolysis and Mineralization

Within the model, hydrolysis is defined as the process by which particulate organic substances are converted to dissolved organic form. Mineralization is defined as the process by which dissolved organic substances are converted to dissolved inorganic form. Conversion of particulate organic phosphorus to phosphate proceeds through the sequence of hydrolysis and mineralization. Direct mineralization of particulate organic phosphorus does not occur.

Mineralization of organic phosphorus is mediated by the release of nucleotidase and phosphatase enzymes by bacteria (Ammerman and Azam 1985; Chrost and Overbeck 1987) and algae (Matavulj and Flint 1987; Chrost and Overbeck 1987; Boni et al. 1989). Since the algae themselves release the enzyme and since bacterial abundance is related to algal biomass, the rate of organic phosphorus mineralization is related, in the model, to algal biomass. A most remarkable property of the enzyme process is that alkaline phosphatase activity is inversely proportional to ambient phosphate concentration (Chrost and Overbeck 1987; Boni et al. 1989). Put in different terms, when phosphate is scarce, algae stimulate production of an enzyme that mineralizes organic phosphorus to phosphate. This phenomenon is simulated by relating mineralization to the algal phosphorus nutrient limitation. Mineralization is highest when algae are strongly phosphorus limited and is least when no limitation occurs.

The expression for mineralization rate is:

$$Kdop = Kdp + \frac{KHp}{KHp + PO_4} \bullet Kdpalg \bullet B$$

Equation 23

in which:

Kdop = mineralization rate of dissolved organic phosphorus (d^{-1})
Kdp = minimum mineralization rate (d^{-1})
KHp = half-saturation concentration for algal phosphorus uptake (g P m^{-3})
PO_4 = dissolved phosphate (g P m^{-3})
Kdpalg = constant that relates mineralization to algal biomass (m^3 g^{-1} C d^{-1})

Potential effects of algal biomass and nutrient limitation on the mineralization rate are shown in Figure 10. When nutrient concentration greatly exceeds the half-saturation concentration for algal uptake, the rate roughly equals the minimum. Algal biomass has little influence. As nutrient becomes scarce relative to the half-saturation concentration, the rate increases. The magnitude of the increase depends on algal biomass. Factor of two to three increases are feasible.

Exponential functions (Figure 5) relate mineralization and hydrolysis rates to temperature.

Dissolved Phosphate

The mass-balance equation for dissolved phosphate is:

$$\frac{\delta}{\delta t} PO_4 = Kdop \bullet DOP - APC \bullet G \bullet B + APC \bullet \left[FPI \bullet BM \bullet B + FPIP \bullet PR\right]$$

Equation 24

in which:

FPI = fraction of algal metabolism released as dissolved phosphate ($0 \leq FPI \leq 1$)
FPIP = fraction of predation released as dissolved phosphate ($0 \leq FPIP \leq 1$)

Dissolved Organic Phosphorus

The mass balance equation for dissolved organic phosphorus is:

$$\frac{\delta}{\delta t} DOP = APC \bullet (BM \bullet B \bullet FPD + PR \bullet FPDP) + Klpop \bullet LPOP + Krpop \bullet RPOP - Kdop \bullet DOP$$

Equation 25

in which:

DOP = dissolved organic phosphorus (g P m^{-3})
LPOP = labile particulate organic phosphorus (g P m^{-3})
RPOP = refractory particulate organic phosphorus (g P m^{-3})
FPD = fraction of algal metabolism released as DOP ($0 < FPD < 1$)
FPDP = fraction of predation on algae released as DOP ($0 < FPDP < 1$)
Klpop = hydrolysis rate of LPOP (d^{-1})

Krpop = hydrolysis rate of RPOP (d^{-1})
Kdop = mineralization rate of DOP (d^{-1})

Labile Particulate Organic Phosphorus

The mass balance equation for labile particulate organic phosphorus is:

$$\frac{\delta}{\delta t} LPOP = APC \bullet (BM \bullet B \bullet FPL + PR \bullet FPLP) - Klpop \bullet LPOP - Wl \bullet \frac{\delta}{\delta z} LPOP$$

Equation 26

in which:

FPL = fraction of algal metabolism released as LPOP ($0 < FPL < 1$)
FPLP = fraction of predation on algae released as LPOP ($0 < FPLP < 1$)

Refractory Particulate Organic Phosphorus

The mass balance equation for refractory particulate organic phosphorus is:

$$\frac{\delta}{\delta t} RPOP = APC \bullet (BM \bullet B \bullet FPR + PR \bullet FPRP) - Krpop \bullet RPOP - Wr \bullet \frac{\delta}{\delta z} RPOP$$

Equation 27

in which:

FPR = fraction of algal metabolism released as RPOP ($0 < FPR < 1$)
FPRP = fraction of predation on algae released as RPOP ($0 < FPRP < 1$)

Nitrogen

The model nitrogen cycle (Figure 11) includes the following processes:

Algal production and metabolism
Predation

Hydrolysis of particulate organic nitrogen
Mineralization of dissolved organic nitrogen
Settling
Nitrification
Denitrification

External loads provide the ultimate source of nitrogen to the system. Available nitrogen is incorporated by algae during growth and released as ammonium and organic nitrogen through respiration and predation. A portion of the particulate organic nitrogen hydrolyzes to dissolved organic nitrogen. The balance settles to the sediments. Dissolved organic nitrogen is mineralized to ammonium. In an oxygenated water column, a fraction of the ammonium is subsequently oxidized to nitrate+nitrite through the nitrification process. In anoxic water, nitrate+nitrite is lost to nitrogen gas through denitrification. Particulate nitrogen that settles to the sediments is mineralized and recycled to the water column, primarily as ammonium. Nitrate+nitrite moves in both directions across the sediment-water interface, depending on relative concentrations in the water column and sediment interstices.

Nitrification

Nitrification is a process mediated by specialized groups of autotrophic bacteria that obtain energy through the oxidation of ammonium to nitrite and oxidation of nitrite to nitrate. A simplified expression for complete nitrification (Tchobanoglous and Schroeder 1987) is:

$$NH_4^+ + 2\ O_2 \rightarrow NO_3^- + H_2O + 2\ H^+$$

Equation 28

The simplified stoichiometry indicates that two moles of oxygen are required to nitrify one mole of ammonium into nitrate. The simplified equation is not strictly true, however. Cell synthesis by nitrifying bacteria is accomplished by the fixation of carbon dioxide so that less than two moles of oxygen are consumed per mole ammonium utilized (Wezernak and Gannon 1968).

The kinetics of complete nitrification are modeled as a function of available ammonium, dissolved oxygen, and temperature:

$$NT = \frac{DO}{KHont + DO} \bullet \frac{NH_4}{KHnnt + NH_4} \bullet f(T) \bullet NTm$$

Equation 29

in which:

NT = nitrification rate (g N m^{-3} d^{-1})
KHont = half-saturation constant of dissolved oxygen required for nitrification (g O_2 m^{-3})
KHnnt = half-saturation constant of NH_4 required for nitrification (g N m^{-3})
NTm = maximum nitrification rate at optimal temperature (g N m^{-3} d^{-1})

The kinetics formulation (Figure 12) incorporates the products of two Monod-like functions. The first function diminishes nitrification at low dissolved oxygen concentration. The second function expresses the influence of ammonium concentration on nitrification. When ammonium concentration is low, relative to KHnnt, nitrification is proportional to ammonium concentration. For NH4 << KHnnt, the reaction is approximately first-order. (The first-order decay constant . NTm/KHnnt.) When ammonium concentration is large, relative to KHnnt, nitrification approaches a maximum rate. This formulation is based on a concept proposed by Tuffey et al. (1974). Nitrifying bacteria adhere to benthic or suspended sediments. When ammonium is scarce, vacant surfaces suitable for nitrifying bacteria exist. As ammonium concentration increases, bacterial biomass increases, vacant surfaces are occupied, and the rate of nitrification increases. The bacterial population attains maximum density when all surfaces suitable for bacteria are occupied. At this point, nitrification proceeds at a maximum rate independent of additional increase in ammonium concentration.

The optimal temperature for nitrification may be less than peak temperatures that occur in temperate waters. To allow for a decrease in nitrification at superoptimal temperature, the effect of temperature on nitrification is modeled in the Gaussian form of Equation 7.

Effect of Denitrification on Nitrate

The effect of denitrification on dissolved organic carbon has been described. Denitrification removes nitrate from the system in stoichiometric proportion to carbon removal:

$$\frac{\delta}{\delta t} NO_3 = - ANDC \ \ Denit \ \ DOC$$

Equation 30

in which:

ANDC = mass nitrate-nitrogen reduced per mass dissolved organic carbon oxidized (0.933 g N g^{-1} C)

Nitrogen Mass Balance Equations

The mass-balance equation for nitrogen state variables are written by summing all previously-described sources and sinks:

Ammonium

$$\frac{\delta}{\delta t} NH_4 = ANC \bullet \left[(BM \bullet FNI - PN \bullet P) \bullet B + PR \bullet FNIP\right] + Kdon \bullet DON - NT$$

Equation 31

in which:

FNI = fraction of algal metabolism released as NH4 ($0 \leq FNI \leq 1$)
PN = algal ammonium preference ($0 \leq PN \leq 1$)
FNIP = fraction of predation released as NH4 ($0 \leq FNIP \leq 1$)

Nitrate+Nitrite

$$\frac{\delta}{\delta t} NO_{23} = - ANC \bullet (1 - PN) \bullet P \bullet B + NT - ANDC \bullet Denit \bullet DOC$$

Equation 32

Dissolved Organic Nitrogen

$$\frac{\delta}{\delta t} DON = ANC \bullet (BM \bullet B \bullet FND + PR \bullet FNDP) + Klpon \bullet LPON + Krpon \bullet RPON - Kdon \bullet DON$$

Equation 33

in which:

DON = dissolved organic nitrogen (g N m^{-3})
LPON = labile particulate organic nitrogen (g N m^{-3})
RPON = refractory particulate organic nitrogen (g N m^{-3})
FND = fraction of algal metabolism released as DON ($0 < FND < 1$)
FNDP = fraction of predation on algae released as DON ($0 < FNDP < 1$)
Klpon = hydrolysis rate of LPON (d^{-1})
Krpon = hydrolysis rate of RPON (d^{-1})
Kdon = mineralization rate of DON (d^{-1})

Labile Particulate Organic Nitrogen

$$\frac{\delta}{\delta t} LPON = ANC \bullet (BM \bullet B \bullet FNL + PR \bullet FNLP) - Klpon \bullet LPON - Wl \bullet \frac{\delta}{\delta z} LPON$$

Equation 34

in which:

FNL = fraction of algal metabolism released as LPON ($0 < FNL < 1$)
FNLP = fraction of predation on algae released as LPON ($0 < FNLP < 1$)

Refractory Particulate Organic Nitrogen

$$\frac{\delta}{\delta t} RPON = ANC \bullet (BM \bullet B \bullet FPR + PR \bullet FPRN) - Krpon \bullet RPON - Wr \bullet \frac{\delta}{\delta z} RPON$$

Equation 35

in which:

FNR = fraction of algal metabolism released as RPON ($0 < FNR < 1$)
FNRP = fraction of predation on algae released as RPON ($0 < FNRP < 1$)

Chemical Oxygen Demand

Chemical oxygen demand is the concentration of reduced substances that are oxidized through abiotic reactions. In the model, chemical oxygen demand originates as methane released from sediments. Methane is quantified in units of oxygen demand and modeled with the following relationship:

$$\frac{\delta}{\delta t} COD = - \frac{DO}{KHocod + DO} \bullet Kcod \bullet COD$$

Equation 36

in which:

COD = chemical oxygen demand concentration (g oxygen-equivalents m^{-3})
KHocod = half-saturation concentration of dissolved oxygen required for exertion of chemical oxygen demand (g O_2 m^{-3})
Kcod = oxidation rate of chemical oxygen demand (d^{-1})

An exponential function (Figure 5) describes the effect of temperature on exertion of chemical oxygen demand.

Dissolved Oxygen

Sources and sinks of dissolved oxygen in the water column (Figure 13) include:

Algal photosynthesis
Atmospheric reaeration
Algal respiration
Heterotrophic respiration
Nitrification
Chemical oxygen demand

Reaeration

The rate of reaeration is proportional to the dissolved oxygen deficit in model segments that form the air-water interface:

$$\frac{\delta}{\delta t} DO = \frac{Kr}{\Delta z} \bullet (DOs - DO)$$

Equation 37

in which:

DO = dissolved oxygen concentration (g O_2 m^{-3})
Kr = reaeration coefficient (m d^{-1})
DOs = dissolved oxygen saturation concentration (g O_2 m^{-3})
Δz = model layer thickness (m)

In freeflowing streams, the reaeration coefficient depends largely on turbulence generated by bottom shear stress (O'Connor and Dobbins 1958). In lakes and coastal waters, however, wind effects may dominate the reaeration process (O'Connor 1983). For Lake Washington, a relationship for wind-driven gas exchange (Hartman and Hammond 1985) was employed:

$$Kr = Arear \bullet Rv \bullet Wms^{1.5}$$

Equation 38

in which:

Arear = empirical constant (. 0.1)
Rv = ratio of kinematic viscosity of pure water at 20 ^{o}C to kinematic viscosity of water at specified temperature and salinity
Wms = wind speed measured at 10 m above water surface (m s^{-1})

Hartman and Hammond (1985) indicate Arear takes the value 0.157. In the present model, Arear is treated as a variable to allow for effects of wind sheltering, for differences in height of local wind observations, and for other factors.

An empirical function (Figure 14) that fits tabulated values of Rv is:

$$Rv = 0.54 + 0.0233 \bullet T - 0.0020 \bullet S$$

Equation 39

in which:

S = salinity (ppt)
T = temperature (^{o}C)

Saturation dissolved oxygen concentration diminishes as temperature and salinity increase. An empirical formula that describes these effects (Genet et al. 1974) is:

$$DOs = 14.5532 - 0.38217 \bullet T + 0.0054258 \bullet T^2$$
$$- CL \bullet (1.665 \times 10^{-4} - 5.866 \times 10^{-6} \bullet T + 9.796 \times 10^{-8} \bullet T^2)$$

Equation 40

in which:

CL = chloride concentration (= salinity/1.80655)

Mass Balance Equation for Dissolved Oxygen

$$\frac{\delta}{\delta t} DO = AOCR \bullet \left[(1.3 - 0.3 \bullet PN) \bullet P - (1 - FCD) \bullet BM\right] \bullet B$$
$$- AONT \bullet NT - \frac{DO}{KHodoc + DO} \bullet AOCR \bullet Kdoc \bullet DOC$$
$$- \frac{DO}{KHocod + DO} \bullet Kcod \bullet COD + \frac{Kr}{H} \bullet (DOs - DO)$$

Equation 41

in which:

AOCR = oxygen-to-carbon mass ratio in production and respiration (= 2.67 g O_2 g^{-1} C)
AONT = oxygen consumed per mass ammonium nitrified (= 4.33 g O_2 g^{-1} N)

Temperature

Computation of temperature employs a conservation of internal energy equation that is analogous to the conservation of mass equation. For practical purposes, the internal energy equation can be written as a conservation of temperature equation. The only source or sink of temperature considered is exchange with the atmosphere. Atmospheric exchange is considered proportional to the temperature difference between the water surface and a theoretical equilibrium temperature (Edinger et al. 1974):

$$\frac{\delta}{\delta t} T = \frac{KT}{\rho \bullet Cp \bullet H} \bullet (Te - T)$$

Equation 42

in which:

T = water temperature (^oC)
Te = equilibrium temperature (^oC)
KT = Heat exchange coefficient (watt m^{-2} $^oC^{-1}$)
Cp = specific heat of water (4200 watt s kg^{-1} $^oC^{-1}$)
ρ = density of water (1000 kg m^{-3})
H = thickness of model surface layer

Inorganic (Fixed) Solids

The only kinetics transformation of fixed solids is settling:

$$\frac{\delta}{\delta t} ISS = - Wiss \bullet \frac{\delta}{\delta z} ISS$$

Equation 43

in which:

ISS = fixed solids concentration (g m^{-3})
Wiss = solids settling velocity (m d^{-1})

Silica

Silica was not activated in the Lake Washington application. The model silica cycle is described here for use in alternate applications. The model incorporates two siliceous state variables, dissolved silica and particulate biogenic silica. The silica cycle (Figure 15) is a simple one in which diatoms take up dissolved silica and recycle dissolved and particulate biogenic silica through the actions of metabolism and predation. Particulate silica dissolves in the water column or settles to the bottom. A portion of the settled particulate biogenic silica dissolves within the sediments and returns to the water column as dissolved silica. Sources and sinks represented are:

Diatom production and metabolism
Predation
Dissolution of particulate to dissolved silica
Settling

Diatoms are conventionally assigned as one of the three algal groups. The model code allows each group to participate in the silica cycle, however. The user has flexibility in assigning the diatom group. The potential also exists to name multiple diatom groups or groups of mixed algae comprised of diatoms and other groups.

Dissolved Silica

The kinetics equation for dissolved silica is:

$$\frac{\delta}{\delta t} Dsil = \left(FSAP \cdot PR - P\right) \cdot ASC \cdot B + Ksua \cdot PBS$$

Equation 44

in which:

Dsil = dissolved silica (g Si m^{-3})
PBS = particulate biogenic silica (g Si m^{-3})

FSAP = fraction of algal silica made available by predation
(0 ≤ FSAP ≤ 1)
ASC = algal silica-to-carbon ratio (g Si g^{-1} C)
Ksua = particulate silica dissolution rate (d^{-1})

Particulate Biogenic Silica

The kinetics equation for particulate biogenic silica is:

$$\frac{\delta}{\delta t} PBS = \left(BM + \left(1 - FSAP\right) \cdot PR\right) \cdot ASC \cdot B - Wpbs \cdot \frac{\delta}{\delta z} PBS - Ksua \cdot PBS$$

Equation 45

in which:

Wpbs = biogenic silica settling rate (m d^{-1})

An exponential function (Figure 5) describes the effect of temperature on silica dissolution.

Parameter Values

Model parameter evaluation is a recursive process. Parameters are selected from a range of feasible values, tested in the model, and adjusted until satisfactory agreement between predicted and observed variables is obtained. Ideally, the range of feasible values is determined by observation or experiment. For some parameters, however, no observations are available. Then, the feasible range is determined by parameter values employed in similar models or by the judgment of the modeler. A review of parameter values was included in documentation of the first application of this model (Cerco and Cole 1994). Parameters from the initial study were refined, where necessary, for the present model. A complete set of parameter values is provided in Table 2.

Table 1
Lake Washington Water Quality Model State Variables

Temperature	Fixed Solids
Phytoplankton	Fecal Coliform
Dissolved Organic Carbon	Labile Particulate Organic Carbon
Refractory Particulate Organic Carbon	Ammonium
Nitrate+Nitrite	Dissolved Organic Nitrogen
Labile Particulate Organic Nitrogen	Refractory Particulate Organic Nitrogen
Total Phosphate	Dissolved Organic Phosphorus
Labile Particulate Organic Phosphorus	Refractory Particulate Organic Phosphorus
Chemical Oxygen Demand	Dissolved Oxygen
Toxicant One	Toxicant Two

Table 2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
AANOX	ratio of anoxic to oxic respiration	0.5	$0 \leq AANOX \leq 1$
ANC	nitrogen-to-carbon ratio of algae	0.15	g N g^{-1} C
AOCR	dissolved oxygen-to-carbon ratio in respiration	2.67	g O_2 g^{-1} C
AONT	mass dissolved oxygen consumed per mass ammonium nitrified	4.33	g O_2 g^{-1} N
APC	algal phosphorus-to-carbon ratio	0.0165	g P g^{-1} C
Areaer	empirical constant in reaeration equation	0.08	
BM	basal metabolic rate of algae at reference temperature Tr	0.03	d^{-1}
BPR	base predation rate	0.22 (May – Oct.), 0.045 otherwise	d^{-1}
CChl	carbon-to-chlorophyll ratio	50	g C g^{-1} chl
FCD	fraction of dissolved organic carbon produced by algal metabolism	0.0	$0 \leq FCD \leq 1$
FCDP	fraction of dissolved organic carbon produced by predation	0.6	$0 \leq FCDP \leq 1$
FCL	fraction of labile particulate carbon produced by algal metabolism	0.0	$0 \leq FCL \leq 1$
FCLP	fraction of labile particulate carbon produced by predation	0.12	$0 \leq FCLP \leq 1$
FCR	fraction of refractory particulate carbon produced by algal metabolism	0.0	$0 \leq FCR \leq 1$
FCRP	fraction of refractory particulate carbon produced by predation	0.28	$0 \leq FCRP \leq 1$
FNI	fraction of inorganic nitrogen produced by algal metabolism	0.6	$0 \leq FNI \leq 1$
FNIP	fraction of inorganic nitrogen produced by predation	0.25	$0 \leq FNIP \leq 1$
FND	fraction of dissolved organic nitrogen produced by algal metabolism	0.3	$0 \leq FND \leq 1$
FNDP	fraction of dissolved organic nitrogen produced by predation	0.35	$0 \leq FNDP \leq 1$
FNL	fraction of labile particulate nitrogen produced by algal metabolism	0.075	$0 \leq FNL \leq 1$

Table 2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
FNLP	fraction of labile particulate nitrogen produced by predation	0.12	$0 \leq FNLP \leq 1$
FNR	fraction of refractory particulate nitrogen produced by algal metabolism	0.075	$0 \leq FNR \leq 1$
FNRP	fraction of refractory particulate nitrogen produced by predation	0.28	$0 \leq FNRP \leq 1$
FPD	fraction of dissolved organic phosphorus produced by algal metabolism	0.2	$0 \leq FPD \leq 1$
FPDP	fraction of dissolved organic phosphorus produced by predation	0.2	$0 \leq FPDP \leq 1$
FPI	fraction of dissolved inorganic phosphorus produced by algal metabolism	0.4	$0 \leq FPI \leq 1$
FPIP	fraction of dissolved inorganic phosphorus produced by predation	0.5	$0 \leq FPIP \leq 1$
FPL	fraction of labile particulate phosphorus produced by algal metabolism	0.2	$0 \leq FPL \leq 1$
FPLP	fraction of labile particulate phosphorus produced by predation	0.09	$0 \leq FPLP \leq 1$
FPR	fraction of refractory particulate phosphorus produced by algal metabolism	0.2	$0 \leq FPR \leq 1$
FPRP	fraction of refractory particulate phosphorus produced by predation	0.21	$0 \leq FPRP \leq 1$
Kcod	oxidation rate of chemical oxygen demand	0.1	d^{-1}
Kdoc	dissolved organic carbon respiration rate	0.0075	d^{-1}
Kdon	dissolved organic nitrogen mineralization rate	0.018	d^{-1}
Kdp	minimum mineralization rate of dissolved organic phosphorus	0.12	d^{-1}
Kdpalg	constant that relates mineralization rate to algal biomass	0.2	$m^3\ g^{-1}\ C\ d^{-1}$
KHn	half-saturation concentration for nitrogen uptake by algae	0.025	$g\ N\ m^{-3}$
KHndn	half-saturation concentration of nitrate required for denitrification	0.1	$g\ N\ m^{-3}$
KHnnt	half-saturation concentration of NH_4 required for nitrification	1.0	$g\ N\ m^{-3}$
KHocod	half-saturation concentration of dissolved oxygen required for exertion of COD	0.5	$g\ O_2\ m^{-3}$
KHodoc	half-saturation concentration of dissolved oxygen required for oxic respiration	0.5	$g\ O_2\ m^{-3}$

Table 2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
KHont	half-saturation concentration of dissolved oxygen required for nitrification	3.0	g O_2 m^{-3}
KHp	half-saturation concentration for phosphorus uptake by algae	0.005	g P m^{-3}
Klpoc	labile particulate organic carbon dissolution rate	0.005	d^{-1}
Klpon	labile particulate organic nitrogen hydrolysis rate	0.08	d^{-1}
Klpop	labile particulate organic phosphorus hydrolysis rate	0.1	d^{-1}
Krpoc	refractory particulate organic carbon dissolution rate	0.001	d^{-1}
Krpon	refractory particulate organic nitrogen hydrolysis rate	0.001	d^{-1}
Krpop	refractory particulate organic phosphorus hydrolysis rate	0.001	d^{-1}
KTb	effect of temperature on basal metabolism of algae	0.032	$^oC^{-1}$
KTcod	effect of temperature on exertion of chemical oxygen demand	0.041	d^{-1}
KTg1	effect of temperature below Tm on growth of algae	0.003	$^oC^{-2}$
KTg2	effect of temperature above Tm on growth of algae	0.01	$^oC^{-2}$
KThdr	effect of temperature on hydrolysis rates	0.069	$^oC^{-1}$
KTmnl	effect of temperature on mineralization rates	0.069	$^oC^{-1}$
KTnt1	effect of temperature below Tmnt on nitrification	0.001	$^oC^{-2}$
KTnt2	effect of temperature above Tmnt on nitrification	0.001	$^oC^{-2}$
NTm	maximum nitrification rate at optimal temperature	0.075	g N m^{-3} d^{-1}
Pm^B	maximum photosynthetic rate	250	g C g^{-1} Chl d^{-1}
Presp	photo-respiration fraction	0.25	$0 \leq Presp \leq 1$
Topt	optimal temperature for growth of algae	25	^oC
Tmnt	optimal temperature for nitrification	30	^oC
Tr	reference temperature for metabolism	20	^oC
Trhdr	reference temperature for hydrolysis	20	^oC

Table 2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
Trmnl	reference temperature for mineralization	20	^{o}C
Wa	algal settling rate	0.1	$m\ d^{-1}$
Wl	settling velocity of labile particles	0.8	$m\ d^{-1}$
Wr	settling velocity of refractory particles	0.8	$m\ d^{-1}$
Wiss	settling velocity of fixed solids	1.0	$m\ d^{-1}$
α	initial slope of production vs. irradiance relationship	8.0	$g\ C\ g^{-1}$ Chl $(E\ m^{-2})^{-1}$

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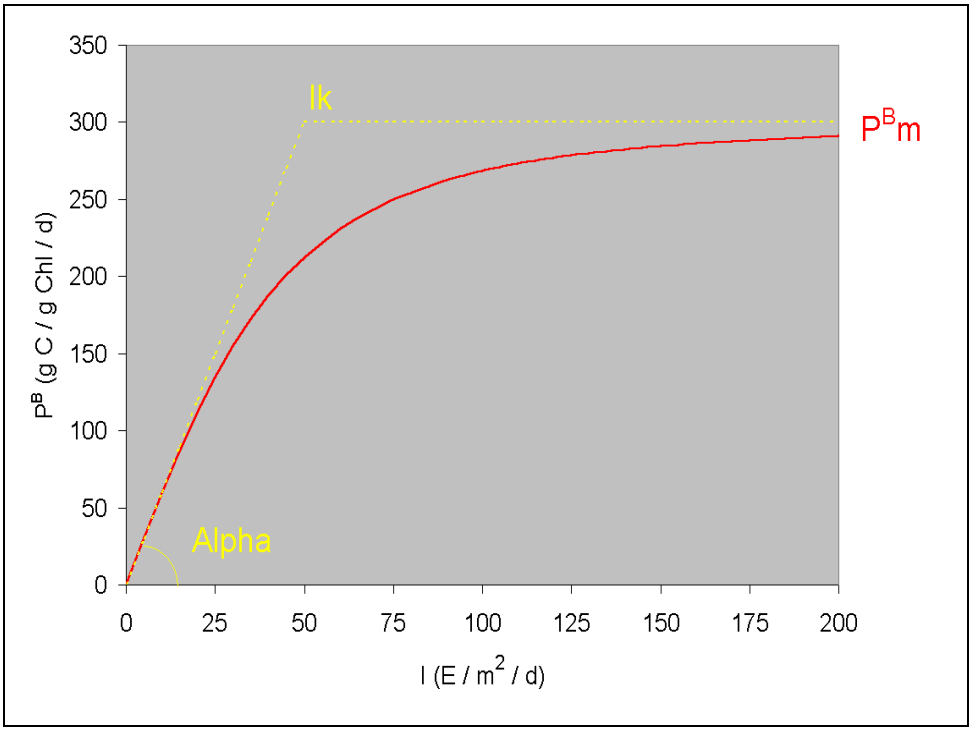

Figure 1. Production versus irradiance curve

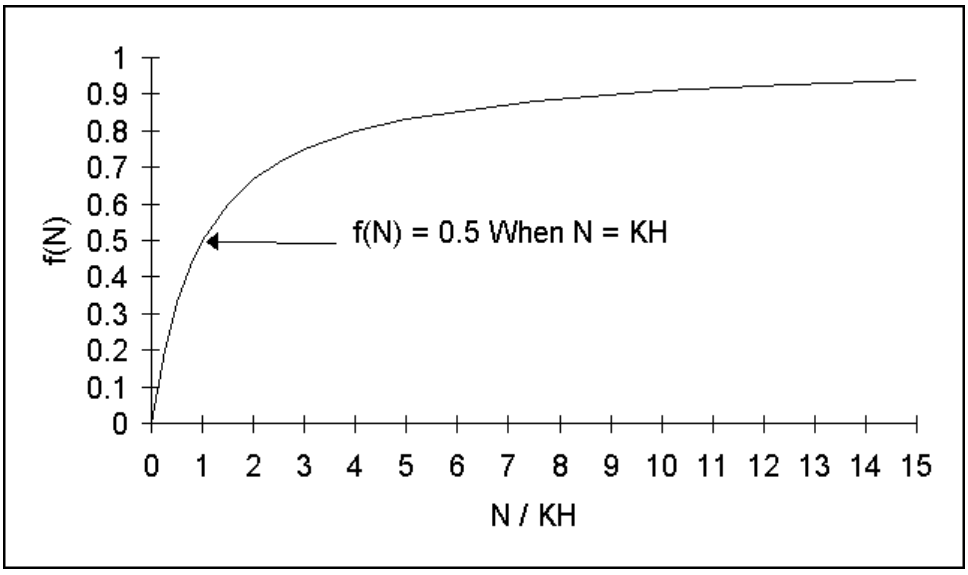

Figure 2. Michaelis-Menton formulation for nutrient-limited growth

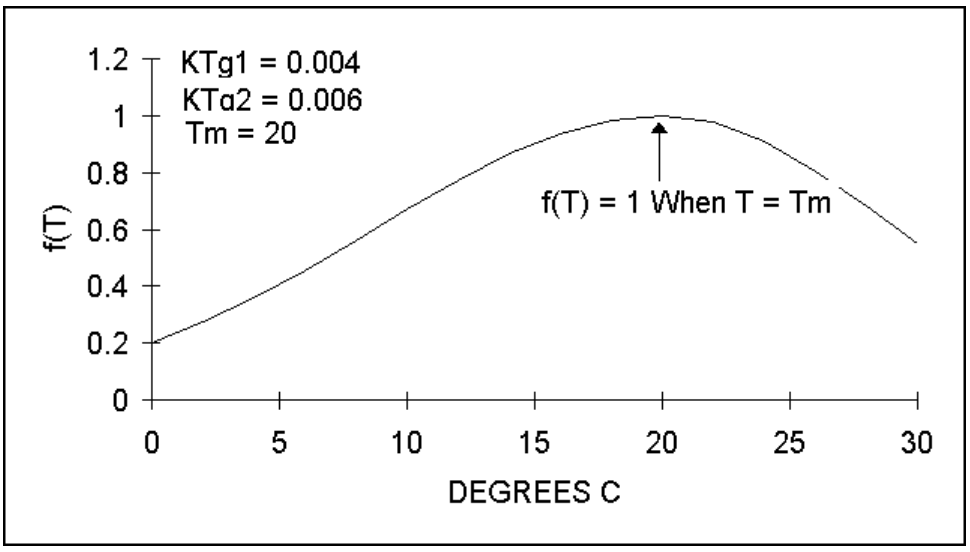

Figure 3. Relation of algal production to temperature

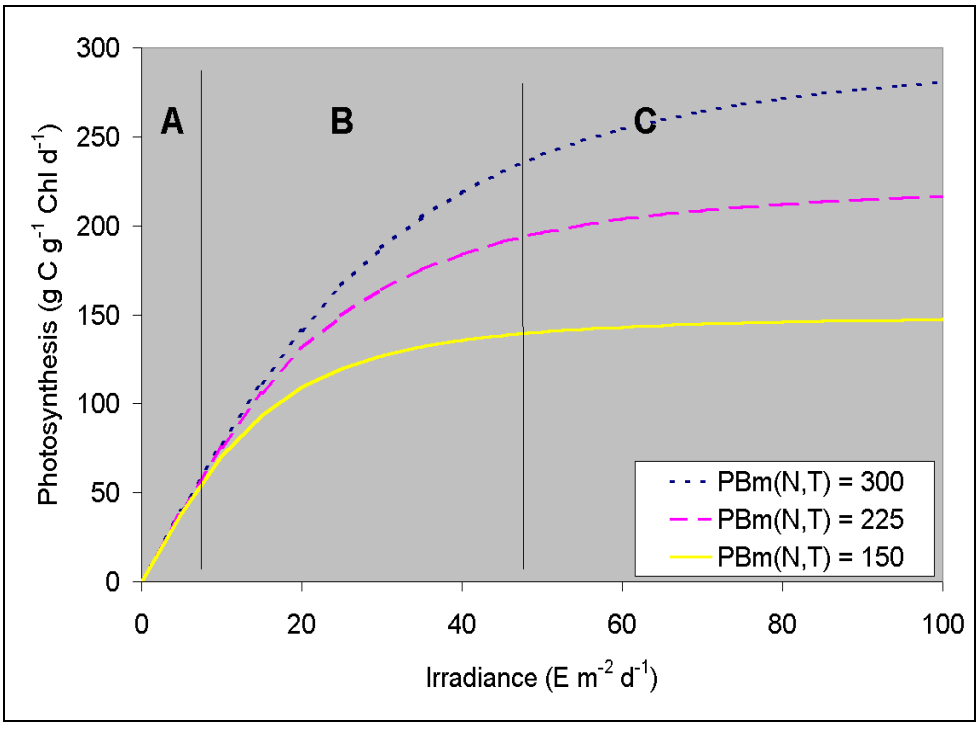

Figure 4. Effects of light and nutrients on production versus irradiance curve, calculated for α = 8 (g C g^{-1} Chl (E m^{-2})$^{-1}$)

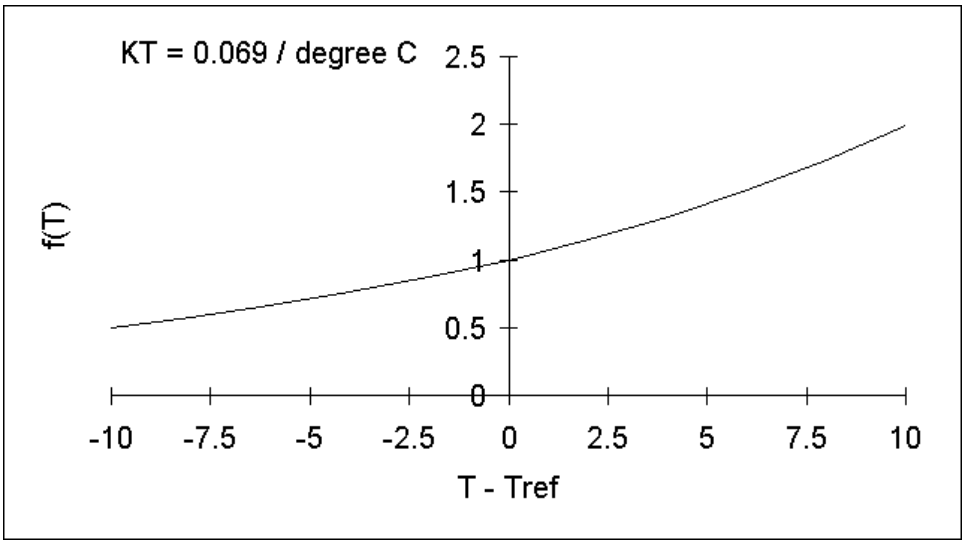

Figure 5. Exponential temperature relationship employed for metabolism and other processes

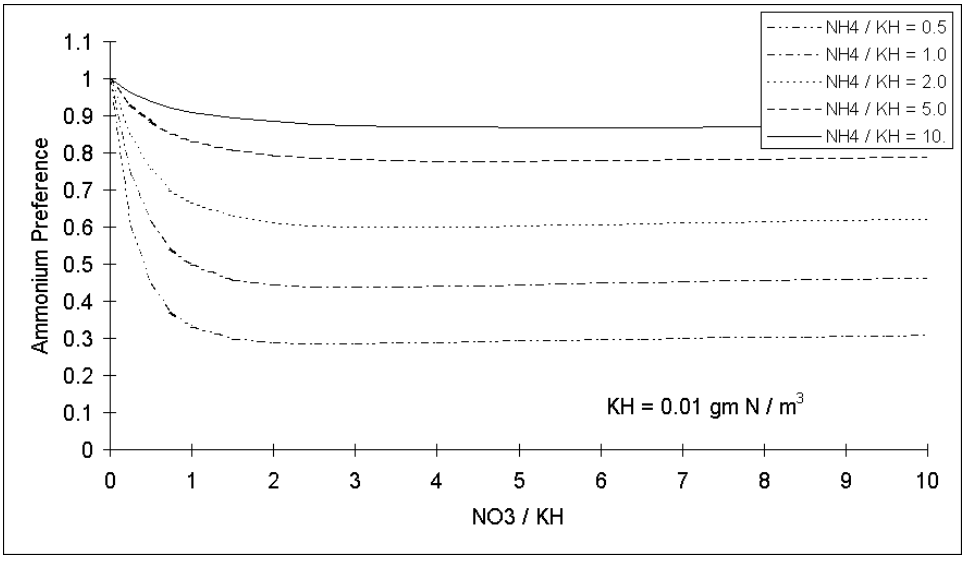

Figure 6. Algal ammonium preference

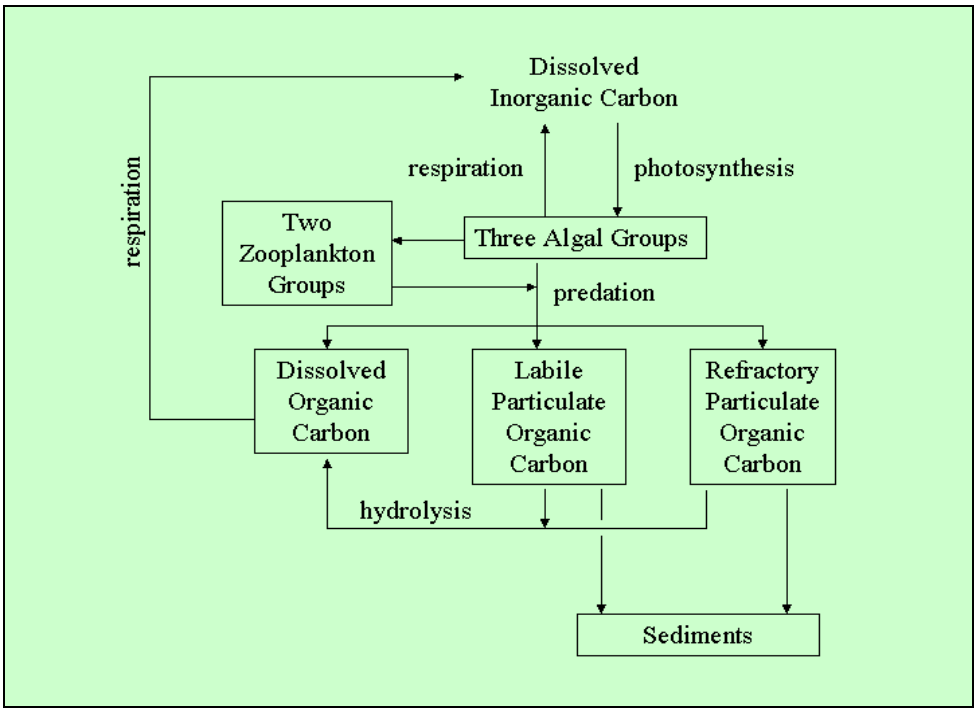

Figure 7. Model carbon cycle

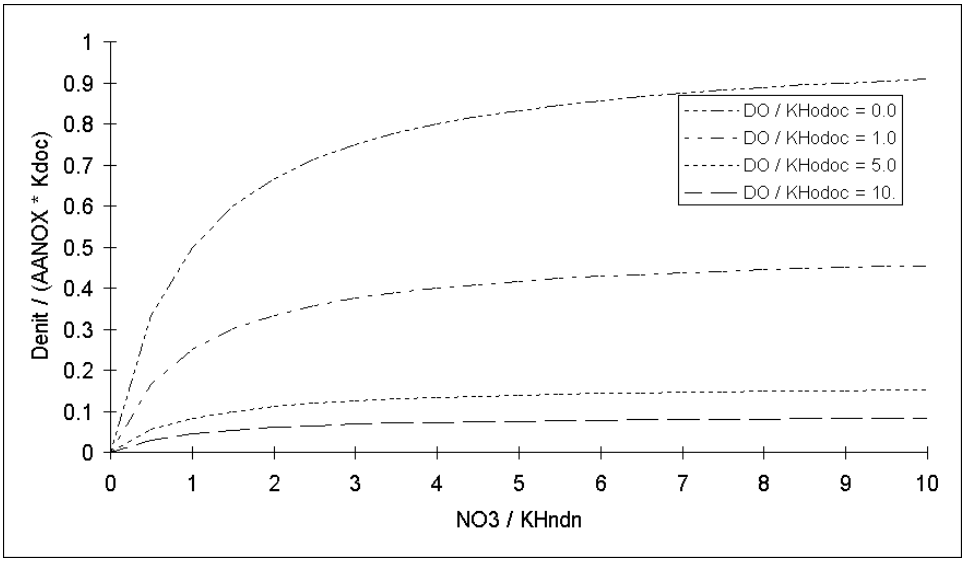

Figure 8. Effect of dissolved oxygen and nitrate on denitrification

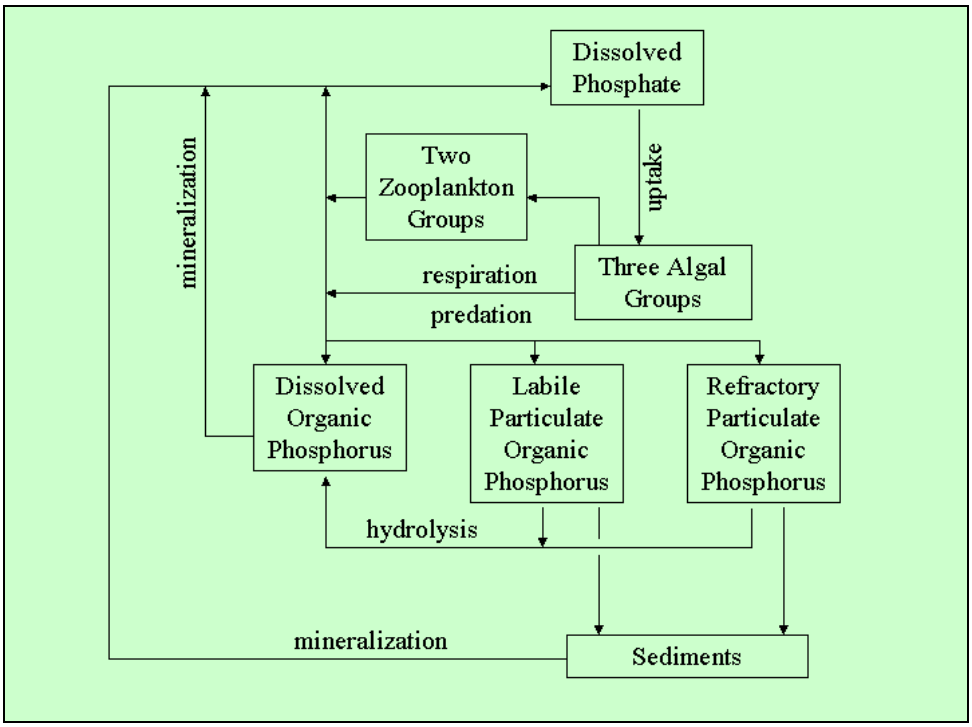

Figure 9. Model phosphorus cycle

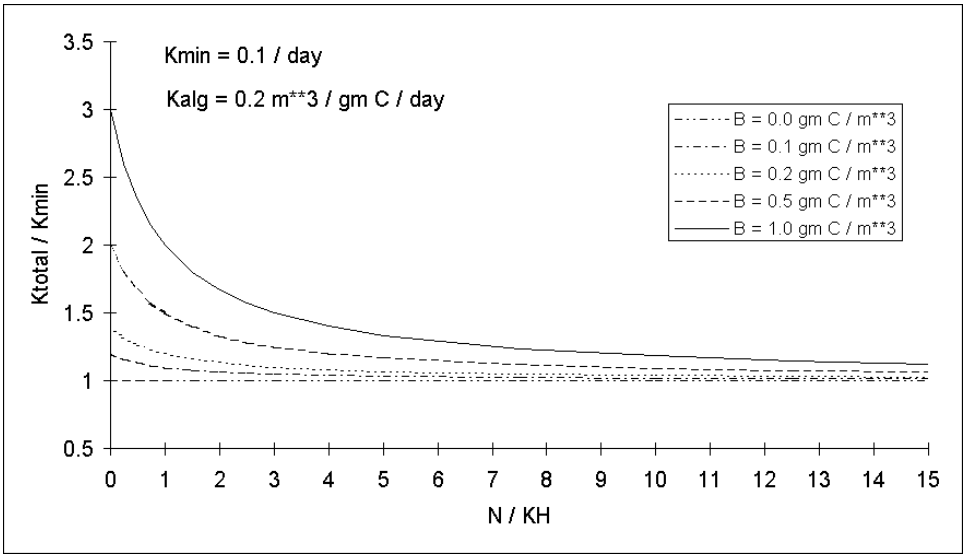

Figure 10. Effect of algal biomass and nutrient concentration on phosphorus mineralization

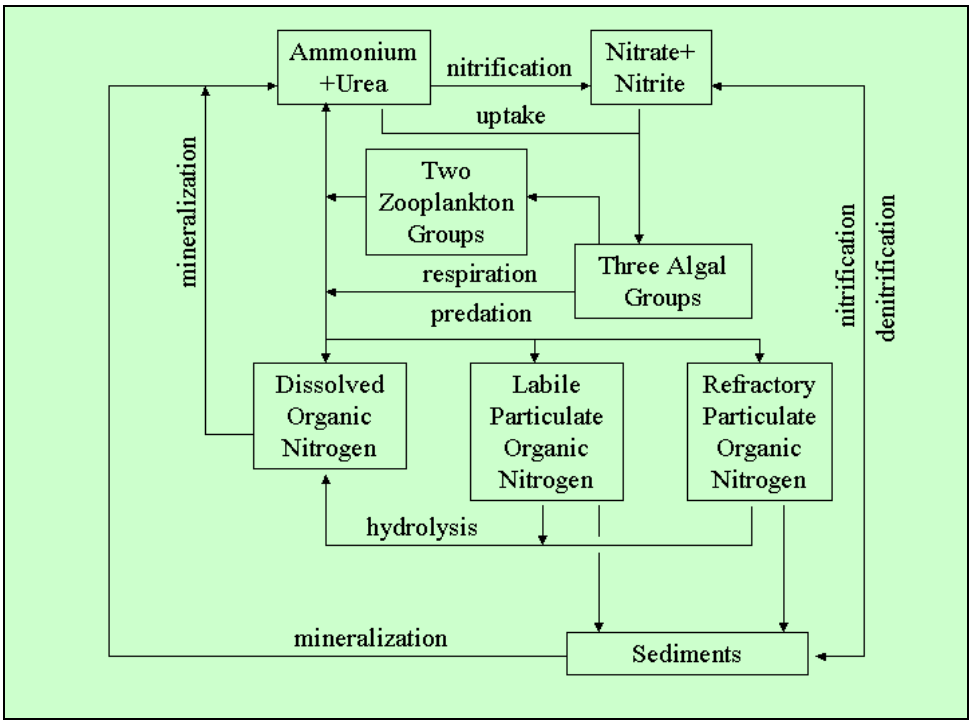

Figure 11. Model nitrogen cycle

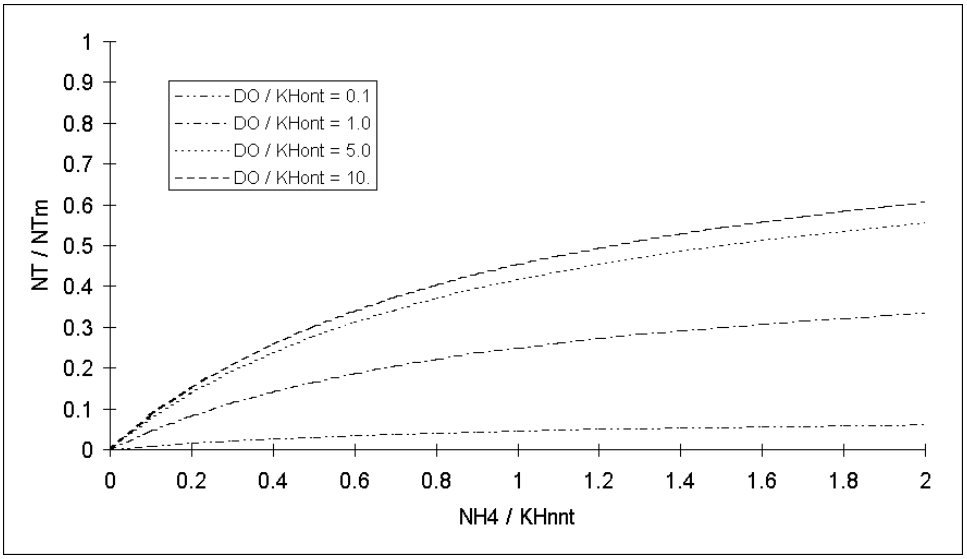

Figure 12. Effect of dissolved oxygen and ammonium concentrations on nitrification rate

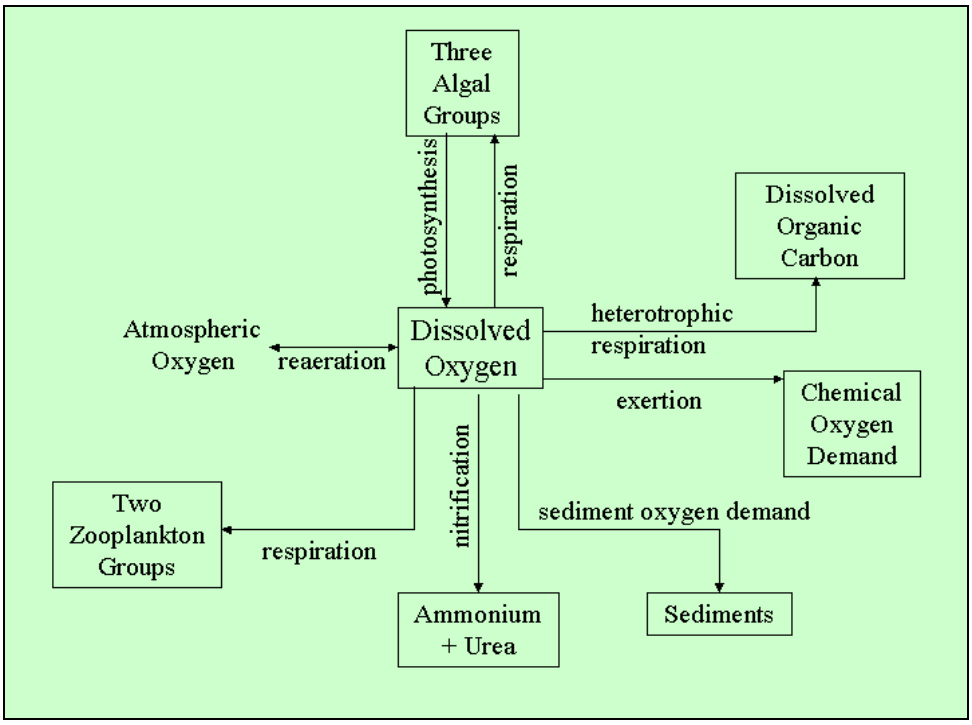

Figure 13. Dissolved oxygen sources and sinks

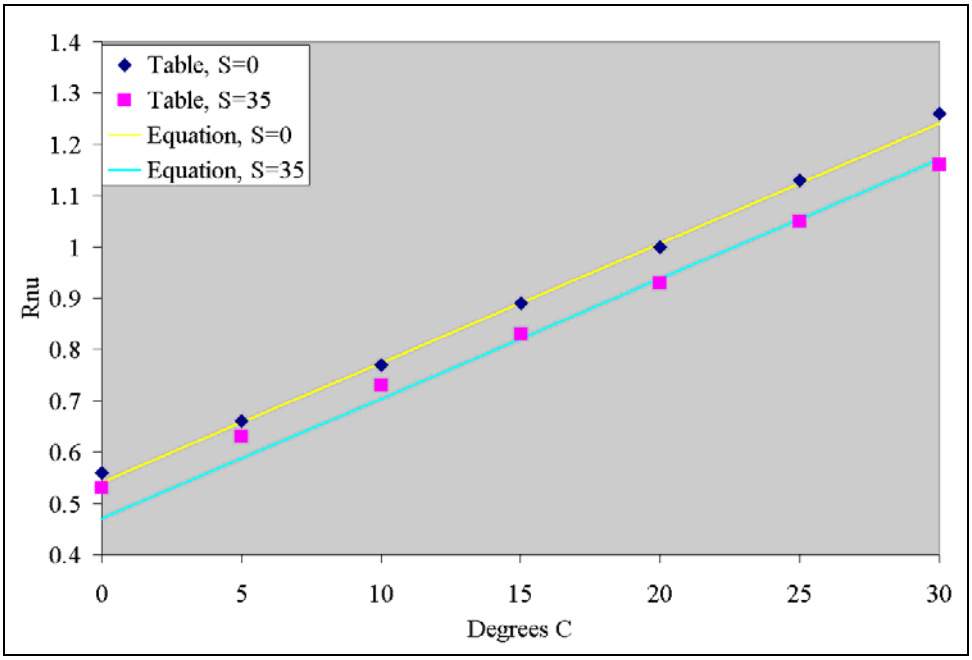

Figure 14. Computed and tabulated values of Rv

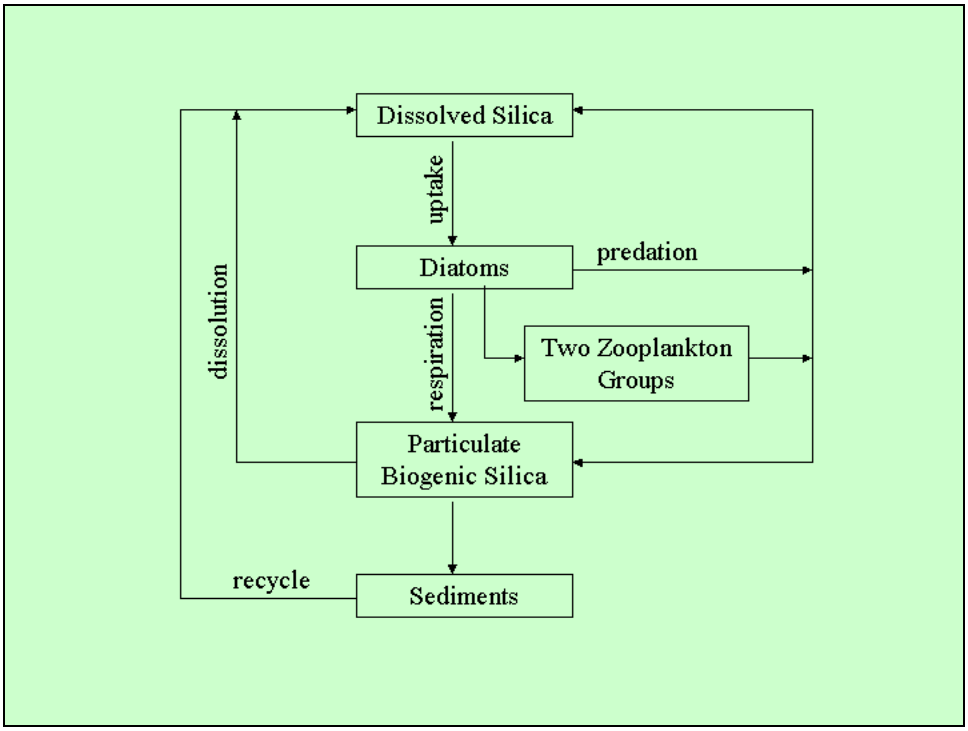

Figure 15. The model silica cycle

The Mineralization Rates File

The Mineralization Rates File contains three sections. These are a title, a section of spatially-uniform parameters, and a section of spatially-varying parameters.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe mineralization rates deck

Two title lines are required to describe the mineralization rates deck. These are not read as variables but are skipped by a FORMAT statement.

Example

```
MINERIZATION RATES FOR NEW GRID WITH PvsI KINETICS.  FEB 10, 2000
Include ANDC, previously omitted
```

Spatially-Uniform Parameters

Each group of the spatially-uniform parameters follows the same convention – a blank line, a parameter list, and a line of parameter values. The format for each group is (//(8X,9F8.0)).

Field	Name	Value	Description
1	KHONT	Real	Half-saturation concentration of dissolved oxygen required for nitrification (g DO m^{-3})
2	KHNNT	Real	Half-saturation concentration of ammonium required for nitrification (g N m^{-3})
3	KHOCOD	Real	Half-saturation concentration of dissolved oxygen required for COD exertion (g DO m^{-3})
4	KHODOC	Real	Half-saturation concentration of dissolved oxygen required for DOC oxidation (g DO m^{-3})
5	KHNDN	Real	Half-saturation concentration of nitrate required for denitrification (g DO m^{-3})

1	AOCR	Real	Mass ratio of oxygen consumed per unit carbon oxidized (g O_2 g^{-1} C)
2	AONT	Real	Mass ratio of oxygen consumed per unit nitrogen nitrified (g O_2 g^{-1} N)
1	TRCOD	Real	Reference temperature for specification of COD oxidation rate (^oC)
2	TRMNL	Real	Reference temperature for specification of dissolved organic matter mineralization rates (^oC)
3	TRHDR	Real	Reference temperature for specification of particulate organic matter hydrolysis rates (^oC)
4	TRSUA	Real	Reference temperature for specification of particulate biogenic silica dissolution rate (^oC)
1	KTCOD	Real	Effect of temperature on COD exertion ($^oC^{-1}$)
2	KTMNL	Real	Effect of temperature on dissolved organic matter mineralization rates ($^oC^{-1}$)
3	KTHDR	Real	Effect of temperature on particulate organic matter hydrolysis rates ($^oC^{-1}$)
4	KTSUA	Real	Effect of temperature on particulate biogenic silica dissolution rates ($^oC^{-1}$)
1	KTNT1	Real	Effect of sub-optimal temperature on nitrification ($^oC^{-2}$)
2	KTNT2	Real	Effect of super-optimal temperature on nitrification ($^oC^{-2}$)
3	TMNT	Real	Optimal temperature for nitrification (^oC)
1	KADPO4	Real	Partition coefficient for sorption of phosphate on inorganic solids (m^3 g^{-1} solids)
2	KADSA	Real	Partition coefficient for sorption of silica on inorganic solids (m^3 g^{-1} solids)
1	AANOX	Real	Ratio of rate of aerobic organic matter oxidation to rate of anaerobic oxidation
2	ANDC	Real	Mass ratio of nitrate consumed per unit organic carbon oxidized via denitrification (g N g^{-1} C)
1	AREAR	Real	Empirical constant in reaeration equation (≈0.1)
2	BREAR	Real	Ratio of windspeed over water to windspeed at measurement location
3	BREAR	Real	Exponent of windspeed in reaeration equation

Example

```
HALF SAT   KHONT   KHNNT  KHOCOD  KHODOC   KHNDN
             3.0     1.0   0.500     0.5     0.1

RATIOS      AOCR    AONT
            2.67    4.33

REF T RESP TRCOD   TRMNL   TRHDR   TRSUA
            23.0    20.0    20.0    20.0

TEMP EFF   KTCOD   KTMNL   KTHDR   KTSUA
           0.041   0.069   0.069   0.092

NITRIF T   KTNT1   KTNT2    TMNT
           0.001   0.001    30.0

SORPTION  KADPO4   KADSA
             0.0     0.0

MISC       AANOX    ANDC
             0.5   0.933

REAER      AREAR   BREAR   CREAR
           0.080     1.5     1.5
```

Spatially-Varying Parameters

Mineralization, hydrolysis, and other rates may be applied uniformly throughout the domain or may be varied spatially. The option to vary these spatially is useful for large systems in which different conditions prevail e.g. freshwater vs. saltwater. Each spatially-varying parameter requires two parameter lists. Each list follows the same convention – a blank line, a parameter list, and a line of parameter values. The first parameter list (//8X,2A8) specifies spatially-uniform or varying parameter assignment and determines if input values should be echoed to the snapshot file. For spatially-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to spatially-varying parameter assignment. At present, the option to print parameter values is disabled. Parameter values are specified in the second parameter list (//:(8X,9F8.0)). One parameter value is required for CONSTANT specification. Otherwise, a value must be entered for each cell in the model grid, nine values to a line. The first field of each line is not read by the program. This field may be used to number input lines for files of extensive size. Parameters are understood to be in order starting from cell 1 up to the highest cell number. The user may elect to hold some parameters constant over the model domain while others are varied spatially.

Field	Name	Value	Description
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KDC	Real	Dissolved organic carbon mineralization rate (d^{-1})

1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KLC	Real	Labile particulate organic carbon mineralization rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KRC	Real	Refractory particulate organic carbon mineralization rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KND	Real	Dissolved organic nitrogen mineralization rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KLN	Real	Labile particulate organic nitrogen hydrolysis rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KRN	Real	Refractory particulate organic nitrogen hydrolysis rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KDP	Real	Dissolved organic phosphorus mineralization rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KLP	Real	Labile particulate organic phosphorus hydrolysis rate (d^{-1})

1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KRP	Real	Refractory particulate organic phosphorus hydrolysis rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KSUA	Real	Particulate biogenic silica dissolution rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KCOD	Real	Chemical oxygen demand oxidation rate (d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KDCALG	Real	Constant that relates DOC respiration to algal biomass ($m^3\ g^{-1}\ C\ d^{-1}$)
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KLCALG	Real	Constant that relates LPOC hydrolysis to algal biomass ($m^3\ g^{-1}\ C\ d^{-1}$)
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KRCALG	Real	Constant that relates RPOC hydrolysis to algal biomass ($m^3\ g^{-1}\ C\ d^{-1}$)
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KDNALG	Real	Constant that relates DON mineralization to algal biomass ($m^3\ g^{-1}\ N\ d^{-1}$)

1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KLNALG	Real	Constant that relates LPON hydrolysis to algal biomass (m^3 g^{-1} N d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KRNALG	Real	Constant that relates RPON hydrolysis to algal biomass (m^3 g^{-1} N d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KDPALG	Real	Constant that relates DOP mineralization to algal biomass (m^3 g^{-1} P d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KLPALG	Real	Constant that relates LPOP hydrolysis to algal biomass (m^3 g^{-1} P d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	KRPALG	Real	Constant that relates RPOP hydrolysis to algal biomass (m^3 g^{-1} P d^{-1})
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	NTMAX	Real	Maximum nitrification rate (g N m^{-3} d^{-1})

Example

```
MINERIZATION RATES FOR NEW GRID WITH PvsI KINETICS.  FEB 10, 2000
Include ANDC, previously omitted

HALF SAT   KHONT   KHNNT  KHOCOD  KHODOC   KHNDN
             3.0     1.0   0.500     0.5     0.1

RATIOS      AOCR    AONT
            2.67    4.33

REF T RESP TRCOD   TRMNL   TRHDR   TRSUA
            23.0    20.0    20.0    20.0

TEMP EFF   KTCOD   KTMNL   KTHDR   KTSUA
           0.041   0.069   0.069   0.092

NITRIF T   KTNT1   KTNT2    TMNT
           0.001   0.001    30.0

SORPTION  KADPO4   KADSA
             0.0     0.0

MISC       AANOX    ANDC
             0.5   0.933

REAER      AREAR   BREAR   CREAR
           0.080     1.5     1.5

         SPVARM  PRINTM
        CONSTANT      NO

             KDC     KDC     KDC     KDC     KDC     KDC     KDC     KDC     KDC
       1  0.0075  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

         SPVARM  PRINTM
        CONSTANT      NO

             KLC     KLC     KLC     KLC     KLC     KLC     KLC     KLC     KLC
       1  0.0050  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

         SPVARM  PRINTM
        CONSTANT      NO

             KRC     KRC     KRC     KRC     KRC     KRC     KRC     KRC     KRC
       1  0.0010  5.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

         SPVARM  PRINTM
        CONSTANT      NO

             KND     KND     KND     KND     KND     KND     KND     KND     KND
       1  0.0180  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

         SPVARM  PRINTM
        CONSTANT      NO

             KLN     KLN     KLN     KLN     KLN     KLN     KLN     KLN     KLN
       1  0.0800  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

         SPVARM  PRINTM
        CONSTANT      NO

             KRN     KRN     KRN     KRN     KRN     KRN     KRN     KRN     KRN
       1  0.0010  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

         SPVARM  PRINTM
        CONSTANT      NO

             KDP     KDP     KDP     KDP     KDP     KDP     KDP     KDP     KDP
       1  0.1200  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
```

```
   SPVARM  PRINTM
 CONSTANT      NO

      KLP     KLP     KLP     KLP     KLP     KLP     KLP     KLP     KLP
1  0.1000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

      KRP     KRP     KRP     KRP     KRP     KRP     KRP     KRP     KRP
1  0.0010  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

     KSUA    KSUA    KSUA    KSUA    KSUA    KSUA    KSUA    KSUA    KSUA
1  0.1000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

     KCOD    KCOD    KCOD    KCOD    KCOD    KCOD    KCOD    KCOD    KCOD
1  0.1000  00.000  00.000  00.000  00.000  00.000  00.000  00.000  00.000

   SPVARM  PRINTM
 CONSTANT      NO

   KDCALG  KDCALG  KDCALG  KDCALG  KDCALG  KDCALG  KDCALG  KDCALG  KDCALG
1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

   KLCALG  KLCALG  KLCALG  KLCALG  KLCALG  KLCALG  KLCALG  KLCALG  KLCALG
1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

   KRCALG  KRCALG  KRCALG  KRCALG  KRCALG  KRCALG  KRCALG  KRCALG  KRCALG
1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

   KDNALG  KDNALG  KDNALG  KDNALG  KDNALG  KDNALG  KDNALG  KDNALG  KDNALG
1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

   KLNALG  KLNALG  KLNALG  KLNALG  KLNALG  KLNALG  KLNALG  KLNALG  KLNALG
1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

   KRNALG  KRNALG  KRNALG  KRNALG  KRNALG  KRNALG  KRNALG  KRNALG  KRNALG
1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

   KDPALG  KDPALG  KDPALG  KDPALG  KDPALG  KDPALG  KDPALG  KDPALG  KDPALG
1  0.2000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

   KLPALG  KLPALG  KLPALG  KLPALG  KLPALG  KLPALG  KLPALG  KLPALG  KLPALG
```

```
1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

   KRPALG  KRPALG  KRPALG  KRPALG  KRPALG  KRPALG  KRPALG  KRPALG  KRPALG
1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000

   SPVARM  PRINTM
 CONSTANT      NO

    NTMAX   NTMAX   NTMAX   NTMAX   NTMAX   NTMAX   NTMAX   NTMAX   NTMAX
1  0.0750  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
```

The Algal Growth Rate File

The Algal Growth Rate File contains five sections. These are a title, a section of spatially and temporally constant model parameters, a section of spatially-varying rates, a section that provides the option to apply temporally-varying predation, and a section that provides the option to apply temporally-varying diatom growth.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe Algal Growth Rate file

Six title lines are required to describe the Algal Growth Rate file. These are not read as variables but are skipped by a FORMAT statement.

Example

```
Algal growth rates for 10196-cell grid.
Restore APC = 0.01 for spring, 0.015 for summer
APC is now a constant so that Total P = P + APC*Algae
Total phosphate no longer includes algal phosphorus
No algal kinetics in ocean.  Increase predation in CB1, CB2,
CB3.  A little mortality on Group 1.  Same as SENS49.  3/27/01
```

Constant Parameters

Each parameter group follows the same convention – a blank line, a parameter list, and a line of parameter values. The format for each group is (//(8X,9F8.0)). Parameters must be specified for all three model algal groups, even if all three are not activated.

Usually the recycle fractions for each process, element, and group must sum to unity e.g. FNIP + FNDP + FNRP + FNLP = 1. If they do not sum to unity, mass-balance errors will occur. The group representing the fraction of algal respiration released as organic carbon is an exception. These may sum to less than unity e.g. FCD1 + FCL1 + FCR1 = 0. The remainder is understood to be the fraction representing direct oxygen consumption. For silica, if FSAP < 1, the remainder goes to particulate silica.

As originally applied to Chesapeake Bay, algal group 1 represented freshwater cyanobacteria and group 2 represented spring, saltwater diatoms.

Consequently salinity toxicity terms for these groups are coded so that group 1 mortality occurs at excess salinity while group 2 mortality occurs at low salinity. The code also allows mortality of group 3 at excess salinity although this option is seldom applied.

Field	Name	Value	Description
1	TRPR	Real	Reference temperature for specification of predation (^oC)
2	KTPR	Real	Effect of temperature on predation ($^oC^{-1}$)
1	FNIP	Real	Fraction of algal nitrogen recycled to ammonium via predation ($0 \leq FNIP \leq 1$)
2	FNDP	Real	Fraction of algal nitrogen recycled to the dissolved organic pool via predation ($0 \leq FNDP \leq 1$)
3	FNLP	Real	Fraction of algal nitrogen recycled to the labile particulate pool via predation ($0 \leq FNDP \leq 1$)
4	FNRP	Real	Fraction of algal nitrogen recycled to the refractory particulate pool via predation ($0 \leq FNRP \leq 1$)
1	FPIP	Real	Fraction of algal phosphorus recycled to phosphate via predation ($0 \leq FPIP \leq 1$)
2	FPDP	Real	Fraction of algal phosphorus recycled to the dissolved organic pool via predation ($0 \leq FPDP \leq 1$)
3	FPLP	Real	Fraction of algal phosphorus recycled to the labile particulate pool via predation ($0 \leq FPDP \leq 1$)
4	FPRP	Real	Fraction of algal phosphorus recycled to the refractory particulate pool via predation ($0 \leq FPRP \leq 1$)
1	FDOP	Real	Fraction of algal carbon consumed in direct respiration by predators ($0 \leq FDOP \leq 1$)
2	FCDP	Real	Fraction of algal carbon recycled to the dissolved organic pool via predation ($0 \leq FCDP \leq 1$)
3	FCLP	Real	Fraction of algal carbon recycled to the labile particulate pool via predation ($0 \leq FCDP \leq 1$)
4	FCRP	Real	Fraction of algal carbon recycled to the refractory particulate pool via predation ($0 \leq FCRP \leq 1$)
1	FSAP	Real	Fraction of algal silica recycled to the dissolved pool via predation ($0 \leq FSAP \leq 1$)
1	CCHLA1	Real	Algal group 1 carbon-to-chlorophyll ratio (g C g^{-1} Chl)
2	ANC1	Real	Algal group 1 nitrogen-to-carbon ratio (g N g^{-1} C)

3	APC1	Real	Algal group 1 phosphorus-to-carbon ratio (g N g^{-1} C)
4	ASC1	Real	Algal group 1 silica-to-carbon ratio (g Si g^{-1} C)
5	STF1	Real	Algal group 1 mortality due to high salinity (d^{-1})
1	KHN1	Real	Algal group 1 half-saturation concentration for nitrogen uptake (g N m^{-3})
2	KHP1	Real	Algal group 1 half-saturation concentration for phosphorus uptake (g P m^{-3})
3	KHS1	Real	Algal group 1 half-saturation concentration for silica uptake (g Si m^{-3})
4	KHR1	Real	Dissolved oxygen concentration at which half of respiration is dissolved organic carbon release rather than oxygen consumption (g DO m^{-3})
5	KHST1	Real	Salinity at which salinity mortality is half the maximum value (ppt)
1	ALPHMN	Real	Initial slope of PvsI curve for algal group 1 (g C g^{-1} Chl (E m^{-2})$^{-1}$)
2	PRSP1	Real	Fraction of production consumed in photorespiration for algal group 1 ($0 \leq$ PRSP1 ≤ 1)
1	TMP1	Real	Optimal temperature for algal group 1 production (^{o}C)
2	TR1	Real	Reference temperature for algal group 1 basal metabolism (^{o}C)
1	KTG11	Real	Effect of sub-optimal temperature on algal group 1 production ($^{o}C^{-2}$)
2	KTG12	Real	Effect of super-optimal temperature on algal group 1 production ($^{o}C^{-2}$)
3	KTB1	Real	Effect of temperature on algal group 1 basal metabolism ($^{o}C^{-1}$)
1	FNI1	Real	Fraction of group 1 nitrogen recycled to ammonium via respiration ($0 \leq$ FNI1 ≤ 1)
2	FND1	Real	Fraction of group 2 nitrogen recycled to the dissolved organic pool via respiration ($0 \leq$ FND1 ≤ 1)
3	FNL1	Real	Fraction of group 1 nitrogen recycled to the labile particulate pool via respiration ($0 \leq$ FNL1 ≤ 1)
4	FNR1	Real	Fraction of group 1 nitrogen recycled to the refractory particulate pool via respiration ($0 \leq$ FNR1 ≤ 1)
1	FPI1	Real	Fraction of group 1 phosphorus recycled to phosphate via respiration ($0 \leq$ FPI1 ≤ 1)

2	FPD1	Real	Fraction of group 1 phosphorus recycled to the dissolved organic pool via respiration ($0 \leq FPD1 \leq 1$)
3	FPL1	Real	Fraction of group l phosphorus recycled to the labile particulate pool via respiration ($0 \leq FPL1 \leq 1$)
4	FPR1	Real	Fraction of group 1 phosphorus recycled to the refractory particulate pool via predation ($0 \leq FPR1 \leq 1$)
1	FCD1	Real	Fraction of group 1 respiration released as dissolved organic carbon ($0 \leq FCD1 \leq 1$)
2	FCL1	Real	Fraction of group 1 respiration released as labile particulate carbon ($0 \leq FCD1 \leq 1$)
3	FCR1	Real	Fraction of group 1 respiration released as refractory particulate carbon ($0 \leq FCD1 \leq 1$)
1	CCHLA2	Real	Algal group 2 carbon-to-chlorophyll ratio (g C g^{-1} Chl)
2	ANC2	Real	Algal group 2 nitrogen-to-carbon ratio (g N g^{-1} C)
3	APC2	Real	Algal group 2 phosphorus-to-carbon ratio (g N g^{-1} C)
4	ASC2	Real	Algal group 2 silica-to-carbon ratio (g Si g^{-1} C)
5	STF2	Real	Algal group 2 mortality due to low salinity (d^{-1})
1	KHN2	Real	Algal group 2 half-saturation concentration for nitrogen uptake (g N m^{-3})
2	KHP2	Real	Algal group 2 half-saturation concentration for phosphorus uptake (g P m^{-3})
3	KHS2	Real	Algal group 2 half-saturation concentration for silica uptake (g Si m^{-3})
4	KHR2	Real	Dissolved oxygen concentration at which half of respiration is dissolved organic carbon release rather than oxygen consumption (g DO m^{-3})
5	KHST2	Real	Salinity at which salinity mortality is half the maximum value (ppt)
1	ALPHMN	Real	Initial slope of PvsI curve for algal group 2 (g C g^{-1} Chl $(E\ m^{-2})^{-1}$)
2	PRSP2	Real	Fraction of production consumed in photorespiration for algal group 2 ($0 \leq PRSP2 \leq 1$)

1	TMP2	Real	Optimal temperature for algal group 2 production (^oC)
2	TR2	Real	Reference temperature for algal group 2 basal metabolism (^oC)
1	KTG21	Real	Effect of sub-optimal temperature on algal group 2 production ($^oC^{-2}$)
2	KTG22	Real	Effect of super-optimal temperature on algal group 2 production ($^oC^{-2}$)
3	KTB2	Real	Effect of temperature on algal group 2 basal metabolism ($^oC^{-1}$)
1	FNI2	Real	Fraction of group 2 nitrogen recycled to ammonium via respiration ($0 \leq$ FNI2 ≤ 1)
2	FND2	Real	Fraction of group 2 nitrogen recycled to the dissolved organic pool via respiration ($0 \leq$ FND2 ≤ 1)
3	FNL2	Real	Fraction of group 2 nitrogen recycled to the labile particulate pool via respiration ($0 \leq$ FNL2 ≤ 1)
4	FNR2	Real	Fraction of group 2 nitrogen recycled to the refractory particulate pool via respiration ($0 \leq$ FNR2 ≤ 1)
1	FPI2	Real	Fraction of group 2 phosphorus recycled to phosphate via respiration ($0 \leq$ FPI2 ≤ 1)
2	FPD2	Real	Fraction of group 2 phosphorus recycled to the dissolved organic pool via respiration ($0 \leq$ FPD2 ≤ 1)
3	FPL2	Real	Fraction of group 2 phosphorus recycled to the labile particulate pool via respiration ($0 \leq$ FPL2 ≤ 1)
4	FPR2	Real	Fraction of group 2 phosphorus recycled to the refractory particulate pool via predation ($0 \leq$ FPR2 ≤ 1)
1	FCD2	Real	Fraction of group 2 respiration released as dissolved organic carbon ($0 \leq$ FCD2 ≤ 1)
2	FCL2	Real	Fraction of group 2 respiration released as labile particulate carbon ($0 \leq$ FCD2 ≤ 1)
3	FCR2	Real	Fraction of group 2 respiration released as refractory particulate carbon ($0 \leq$ FCD2 ≤ 1)
1	CCHLA3	Real	Algal group 3 carbon-to-chlorophyll ratio (g C g^{-1} Chl)
2	ANC3	Real	Algal group 3 nitrogen-to-carbon ratio (g N g^{-1} C)
3	APC3	Real	Algal group 3 phosphorus-to-carbon ratio (g N g^{-1} C)

4	ASC3	Real	Algal group 3 silica-to-carbon ratio (g Si g^{-1} C)
5	STF3	Real	Algal group 3 mortality due to high salinity (d^{-1})
1	KHN3	Real	Algal group 3 half-saturation concentration for nitrogen uptake (g N m^{-3})
2	KHP3	Real	Algal group 3 half-saturation concentration for phosphorus uptake (g P m^{-3})
3	KHS3	Real	Algal group 3 half-saturation concentration for silica uptake (g Si m^{-3})
4	KHR3	Real	Dissolved oxygen concentration at which half of respiration is dissolved organic carbon release rather than oxygen consumption (g DO m^{-3})
5	KHST3	Real	Salinity at which salinity mortality is half the maximum value (ppt)
1	ALPHMN	Real	Initial slope of PvsI curve for algal group 3 (g C g^{-1} Chl $(E\ m^{-2})^{-1}$)
2	PRSP3	Real	Fraction of production consumed in photorespiration for algal group 3 ($0 \leq$ PRSP3 ≤ 1)
1	TMP3	Real	Optimal temperature for algal group 3 production (^oC)
2	TR3	Real	Reference temperature for algal group 3 basal metabolism (^oC)
1	KTG31	Real	Effect of sub-optimal temperature on algal group 3 production ($^oC^{-2}$)
2	KTG32	Real	Effect of super-optimal temperature on algal group 3 production ($^oC^{-2}$)
3	KTB3	Real	Effect of temperature on algal group 3 basal metabolism ($^oC^{-1}$)
1	FNI3	Real	Fraction of group 3 nitrogen recycled to ammonium via respiration ($0 \leq$ FNI3 ≤ 1)
2	FND3	Real	Fraction of group 3 nitrogen recycled to the dissolved organic pool via respiration ($0 \leq$ FND3 ≤ 1)
3	FNL3	Real	Fraction of group 3 nitrogen recycled to the labile particulate pool via respiration ($0 \leq$ FNL3 ≤ 1)
4	FNR3	Real	Fraction of group 3 nitrogen recycled to the refractory particulate pool via respiration ($0 \leq$ FNR3 ≤ 1)
1	FPI3	Real	Fraction of group 3 phosphorus recycled to phosphate via respiration ($0 \leq$ FPI3 ≤ 1)

2	FPD3	Real	Fraction of group 3 phosphorus recycled to the dissolved organic pool via respiration ($0 \leq$ FPD3 ≤ 1)
3	FPL3	Real	Fraction of group 3 phosphorus recycled to the labile particulate pool via respiration ($0 \leq$ FPL3 ≤ 1)
4	FPR3	Real	Fraction of group 3 phosphorus recycled to the refractory particulate pool via predation ($0 \leq$ FPR3 ≤ 1)
1	FCD3	Real	Fraction of group 3 respiration released as dissolved organic carbon ($0 \leq$ FCD3 ≤ 1)
2	FCL3	Real	Fraction of group 3 respiration released as labile particulate carbon ($0 \leq$ FCD3 ≤ 1)
3	FCR3	Real	Fraction of group 3 respiration released as refractory particulate carbon ($0 \leq$ FCD3 ≤ 1)

Example

```
PREDATN     TRPR    KTPR
            25.0  0.0000

FRACTN N    FNIP    FNDP    FNLP    FNRP
            0.25    0.30   0.350   0.100

FRACTN P    FPIP    FPDP    FPLP    FPRP
            0.50    0.20   0.200   0.100

FRACTN C    FDOP    FCDP    FCLP    FCRP
            0.00   0.600   0.300   0.100

FRACTN SI   FSAP
             0.3

GROUP 1 1 CCHLA1    ANC1    APC1    ASC1    STF1
             50.   0.175    0.01   0.000    0.30

GROUP 1 2   KHN1    KHP1    KHS1    KHR1   KHST1
            0.02 0.00075    0.00    0.50     0.5

GROUP 1 3 ALPHMN   PRSP1
            3.15    0.25

GROUP 1 4   TMP1     TR1
            29.0   20.00

GROUP 1 5  KTG11   KTG12    KTB1
          0.0050  0.0040  0.0322

GROUP 1 6   FNI1    FND1    FNL1    FNR1
            0.55    0.20   0.200   0.050

GROUP 1 7   FPI1    FPD1    FPL1    FPR1
            0.75    0.25   0.000   0.000

GROUP 1 8   FCD1    FCL1    FCR1
           0.000   0.000   0.000

GROUP 2 1 CCHLA2    ANC2    APC2    ASC2    STF2
             50.   0.175   0.010   0.800     0.1
```

```
GROUP 2 2   KHN2    KHP2    KHS2    KHR2   KHST2
            0.03  0.0030    0.05     0.5     2.0

GROUP 2 3 ALPHMN   PRSP2
            8.00    0.25

GROUP 2 4   TMP2     TR2
            20.0   20.00

GROUP 2 5  KTG21   KTG22    KTB2
         0.00250 0.01200  0.0322

GROUP 2 6   FNI2    FND2    FNL2    FNR2
            0.55    0.20   0.200   0.050

GROUP 2 7   FPI2    FPD2    FPL2    FPR2
            0.70    0.20   0.070   0.030

GROUP 2 8   FCD2    FCL2    FCR2
           0.000   0.000   0.000

GROUP 3 1 CCHLA3    ANC3    APC3    ASC3    STF3
             50.   0.150  0.0165   0.000    0.00

GROUP 3 2   KHN3    KHP3    KHS3    KHR3   KHST3
           0.025   0.005    0.00    0.50    35.0

GROUP 3 3 ALPHMN   PRSP3
            8.00    0.25

GROUP 3 4   TMP3     TR3
            25.0   20.00

GROUP 3 5  KTG31   KTG32    KTB3
         0.00300 0.01000  0.0322

GROUP 3 6   FNI3    FND3    FNL3    FNR3
            0.60    0.25   0.100   0.050

GROUP 3 7   FPI3    FPD3    FPL3    FPR3
            0.40    0.20   0.300   0.100

GROUP 3 8   FCD3    FCL3    FCR3
           0.000   0.000   0.000
```

Spatially-Varying Parameters

Algal production, respiration, and predation losses may be applied uniformly throughout the domain or may be varied spatially. The option to vary these spatially is useful for large systems in which different communities are present e.g. freshwater vs. saltwater. Each group of the spatially-varying parameters follows the same convention – a blank line, a parameter list, and a line of parameter values. The first parameter list (//8X,8A8) specifies spatially-uniform or varying parameter assignment and determines if input values should be echoed to the output file. For spatially-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to spatially-varying parameter assignment. To print entries to the output file, enter the character string ' ALL'. The second parameter list specifies parameter values (//(8X,9F8.0)). One line of parameter values is required for CONSTANT specification. Otherwise, one line must be entered for each cell in the model grid. For convenience, the cell number may be entered in the first eight columns. This number is not read into the program.

Parameters are understood to be in order starting from cell 1 up to the highest cell number.

Field	Name	Value	Description
1	SPVAR1	Character	Spatially uniform (CONSTANT) or varying parameter specification for algal group 1
2	PRINT1	Character	Print (ALL) or do not print out group 1 parameters
1	PM1	Real	Maximum photosynthetic rate for algal group 1 (g C g^{-1} Chl d^{-1})
2	BMR1	Real	Algal group 1 basal metabolism at reference temperature (d^{-1})
3	BPR1	Real	First-order predation rate on algal group 1 (d^{-1})
1	SPVAR2	Character	Spatially uniform (CONSTANT) or varying parameter specification for algal group 2
2	PRINT2	Character	Print (ALL) or do not print out group 2 parameters
1	PM2	Real	Maximum photosynthetic rate for algal group 2 (g C g^{-1} Chl d^{-1})
2	BMR2	Real	Algal group 2 basal metabolism at reference temperature (d^{-1})
3	BPR2	Real	First-order predation rate on algal group 2 (d^{-1})
1	SPVAR3	Character	Spatially uniform (CONSTANT) or varying parameter specification for algal group 3
2	PRINT3	Character	Print (ALL) or do not print out group 3 parameters
1	PM3	Real	Maximum photosynthetic rate for algal group 3 (g C g^{-1} Chl d^{-1})
2	BMR3	Real	Algal group 3 basal metabolism at reference temperature (d^{-1})
3	BPR3	Real	First-order predation rate on algal group 3 (d^{-1})

Example

```
GROUP 1   SPVAR1  PRINT1
        CONSTANT      NO

     BOX      PM1    BMR1    BPR1
       1      0.0   0.030   0.000

GROUP 2   SPVAR2  PRINT2
          CONSTANT      NO

     BOX      PM2    BMR2    BPR2
       1    00.0   0.010   1.000

GROUP 3   SPVAR3  PRINT2
        CONSTANT      NO
```

```
BOX      PM3     BMR3     BPR3
  1    250.0    0.030    1.000
```

Temporally-Varying Predation Rate

Algal predation losses may be multiplied by a constant to create a piecewise predation function. This option is appropriate if predators are present at specific seasons. Each group of the temporally-varying parameters follows the same convention – a blank line, a parameter list, and a line of parameter values. The first parameter list (//8X,8A8) specifies temporally-uniform or varying parameter assignment and determines if input values should be echoed to the output file. For temporally-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to temporally-varying parameter assignment. To print entries to the output file, enter the character string ' ALL'. The second parameter list specifies parameter values (//(16X,F8.0)). One line of parameter values is required for CONSTANT specification. In this case, the value 1.0 should be entered for TVPRSZ or TVPRLZ. Otherwise, 366 lines must be entered – one for each day of the year. For convenience, the day may be entered in the first 16 columns. This number is not read into the program. Parameters are understood to be in order starting from day 1.

This option was employed in Lake Washington to yield higher predation during the summer months. A "trick" was employed in which the base predation rate, BPR3, was specified as unity (1 d^{-1}) and the multiplier was specified as the desired predation rate for each day of the year.

Field	Name	Value	Description
1	TPVAR	Character	Temporally uniform (CONSTANT) or varying parameter specification for predation
2	PRINT	Character	Print (ALL) or do not print out predation multipliers
1	TVPR	Real	Mutiplier applied to base predation rate

Example

```
PREDATN    TPVAR   PRINT
         VARYING     ALL

             DAY    TVPR
               1   0.045
               2   0.045
               3   0.045
               .     .
               .     .
               .     .
             119   0.045
             120   0.045
             121   0.220
             122   0.220
             123   0.220
               .     .
               .     .
               .     .
             297   0.220
             298   0.220
```

```
299   0.220
300   0.045
301   0.045
302   0.045
  .     .
  .     .
  .     .
364   0.045
365   0.045
366   0.045
```

Temporally-Varying Diatom Growth Rate

Chesapeake Bay is characterized by a diatom bloom that commences in late winter and ends precipitously in late spring. Algal group 2 is used to represent these bloom diatoms. The presence of the bloom species is difficult to characterize solely through model parameterization. In particular, if temperature is used to predict the occurrence of the bloom, then a bloom occurs in autumn when temperature is the same as spring. Observations indicate these bloom species are not present in autumn, however. To restrict group 2 production to the months when bloom species are present, a multiplier on the production rate is employed. The multiplier is set to unity during bloom months and zero otherwise. If this feature is not desired, the multiplier can be set to a temporally-constant value of unity.

Each group of the temporally-varying parameters follows the same convention – a blank line, a parameter list, and a line of parameter values. The first parameter list (//8X,8A8) specifies temporally-uniform or varying parameter assignment and determines if input values should be echoed to the output file. For temporally-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to temporally-varying parameter assignment. To print entries to the output file, enter the character string ' ALL'. The second parameter list specifies parameter values (//(16X,F8.0)). One line of parameter values is required for CONSTANT specification. In this case, the value 1.0 should be entered for TB2G2. Otherwise, 366 lines must be entered – one for each day of the year. For convenience, the day may be entered in the first 16 columns. This number is not read into the program. Parameters are understood to be in order starting from day 1.

Field	Name	Value	Description
1	TB2GR	Character	Temporally uniform (CONSTANT) or varying parameter specification for group 2 production
2	PRINT	Character	Print (ALL) or do not print out predation multipliers
1	TB2G2	Real	Mutiplier applied to algal group 2 production rate

Example

```
GROUP 2    TB2GR   PRINT
        CONSTANT     ALL

             DAY   TB2G2
               1    1.00
```

The Settling Rates File

The Settling Rates File contains two sections. These are a title and a section of spatially-varying parameters.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe settling rates file

Two title lines are required to describe the settling rates file. These are not read as variables but are skipped by a FORMAT statement.

Example

```
Settling file for Lake Washington     5/6/02
Halve settling rates for WSS, WLAB, WREF.
```

Spatially-Varying Parameters

Settling rates may be applied uniformly throughout the domain or may be varied spatially. The option to vary these spatially is useful for large systems in which particle properties vary. For example, higher settling rates may be specified near a loading source to indicate rapid settling of large particles. Specification of settling rates requires two parameter lists. Each list follows the same convention – a blank line, a header line, and one or more lines of parameter values. The first parameter list (//8X,2A8) specifies spatially-uniform or varying parameter assignment and determines if input values should be echoed to the snapshot file. For spatially-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to spatially-varying parameter assignment. At present, the option to print parameter values is disabled. Settling rates are specified in the second parameter list (//:(8X,9F8.0)). One line of parameter values is required for CONSTANT specification. Otherwise, a line must be entered for each cell in the model grid, seven values to a line. The first field of each line is not read by the program. This field may be used to number input lines for files of extensive size. Inputs are understood to be in order starting from cell 1 up to the highest cell number.

Field	Name	Value	Description
1	SPVARM	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTM	Character	Print or do not print out parameters (not active)
1	WSS	Real	Fixed solids settling rate (m d^{-1})
2	WSLAB	Real	Labile particulate organic matter settling rate (m d^{-1})
3	WSREF	Real	Refractory particulate organic matter settling rate (m d^{-1})
4	WS1	Real	Algal group 1 settling rate (m d^{-1})
5	WS2	Real	Algal group 2 settling rate (m d^{-1})
6	WS3	Real	Algal group 3 settling rate (m d^{-1})
7	WSPBS	Real	Particulate biogenic silica settling rate (m d^{-1})

Example

```
      SPVARM  PRINTM
    CONSTANT      NO

  BOX     WSS   WSLAB   WSREF     WS1     WS2      WS3   WSPBS
    1   1.000   1.000   1.000   0.000   0.100   0.100   0.100
```

The Light Attenuation File

Light Attenuation

Light attenuation is computed within the model as:

$$KE = KEb + KEISS \cdot ISS + KECHL \cdot CHL + KEDOC \cdot DOC$$

in which:

KE = coefficient of diffuse light attenuation (m^{-1})
KEb = background attenuation (m^{-1})
KEISS = coefficient that relates attenuation to fixed solids concentration ($m^2\ g^{-1}$)
ISS = fixed solids concentration ($g\ m^{-3}$)
KECHL = coefficient that relates attenuation to chlorophyll concentration ($m^2\ mg^{-1}$)
CHL = chlorophyll concentration ($mg\ m^{-3}$)
KEDOC = coefficient that relates attenuation to dissolved organic carbon concentration ($m^2\ g^{-1}$)
DOC = dissolved organic carbon concentration ($g\ m^{-3}$)

Background attenuation represents attenuation from color and other factors not taken into account by fixed solids and chlorophyll. As an alternative, color can be related to dissolved organic carbon concentration. This option is not employed in Lake Washington. Chlorophyll is not a model state variable but is calculated from computed algal carbon and specified carbon-to-chlorophyll ratio. Volatile solids are strongly associated with chlorophyll. Attenuation from volatile solids can be incorporated by increasing the chlorophyll extinction coefficient above the value associated with chlorophyll alone.

The Light Attenuation File contains two sections. These are a title and a section of spatially-varying parameters.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe light attenuation file

Two title lines are required to describe the light attenuation file. These are not read as variables but are skipped by a FORMAT statement.

Example

```
Linear model ke = a + b TSS.  March 7, 2002
KE a linear function of chlorophyll
```

Spatially-Varying Parameters

Light attenuation parameters may be applied uniformly throughout the domain or may be varied spatially. The option to vary these spatially is useful for large systems in which background attenuation or particle properties vary. Specification of light attenuation requires two parameter lists. Each list follows the same convention – a blank line, a header line, and one or more lines of parameter values. The first parameter list (//8X,2A8) specifies spatially-uniform or varying parameter assignment and determines if input values should be echoed to the snapshot file. For spatially-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to spatially-varying parameter assignment. At present, the option to print parameter values is disabled. Attenuation coefficients are specified in the second parameter list (8X,4F8.0). One line of parameter values is required for CONSTANT specification. Otherwise, a line must be entered for each cell in the model grid, four values to a line. The first field of each line is not read by the program. This field may be used to number input lines for files of extensive size. Inputs are understood to be in order starting from cell 1 up to the highest cell number.

Field	Name	Value	Description
1	SPVARKE	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTKE	Character	Print or do not print out parameters (not active)
1	KEB	Real	Background attenuation (m^{-1})
2	KEISS	Real	Coefficient that relates attenuation to fixed solids concentration ($m^2\ g^{-1}$)
3	KECHL	Real	Coefficient that relates attenuation to chlorophyll concentration ($m^2\ mg^{-1}$)
4	KEDOC	Real	Coefficient that relates attenuation to dissolved organic carbon concentration ($m^2\ g^{-1}$)

Example

```
        SPVARKE PRINTKE
       CONSTANT      NO

   CELL     KEB   KEISS   KECHL   KEDOC
      1  0.2900  0.0800  0.0200  0.0000
```

The Zooplankton Model

Introduction

Many of the earliest eutrophication models (e.g. DiToro et al. 1971; DiToro and Matystik 1980) included one or more zooplankton groups as state variables. Later efforts omitted zooplankton (e.g. Thomann and Fitzpatrick 1982). At present, eutrophication models sans zooplankton are widely accepted (e.g. Cerco and Cole 1993). The reasons for dropping zooplankton are unclear. Lack of observations and difficulty in calibration are two possibilities.

Zooplankton were not activated in the initial Lake Washington application. The present chapter details the formulation of zooplankton kinetics and reports parameter values as implemented in Chesapeake Bay. Zooplankton were incorporated into the model during the tributary refinements phase (Cerco, Johnson, and Wang 2002; Cerco and Meyers 2000). The primary reason was to advance the model into the realm of living resources. Although zooplankton have no commercial value, they are a prime food source for commercially-valuable finfish. Addition of zooplankton to the model framework was a first step towards modeling the effects of eutrophication management on top-level predators. A secondary goal of modeling zooplankton was to improve model accuracy in the computation of algal biomass and other parameters.

Model Conceptualization

A conceptual food web for the bay exhibits seven components (Figure 1). At the base of the food web are the phytoplankton. The phytoplankton are preyed upon by zooplankton and by herbivorous finfish (in Chesapeake Bay, menhaden). Dissolved organic carbon (DOC) released from plankton and detritus is consumed by heterotrophic bacteria which, along with phytoplankton, form a food source for the microzooplankton. Microzooplankton are one of the prey groups for the mesozooplankton which also consume phytoplankton and detritus. The mesozooplankton are a primary food source for carnivorous finfish (in Chesapeake Bay, anchovy).

The art in modeling is to determine which of the food web components are to be modeled and to describe the carbon and nutrient transfers between the groups. As the primary producers, the phytoplankton must be modeled. The mesozooplankton are the primary food source for the bay anchovies. Modeling the prey biomass and mass flows into the finfish are among the primary goals of the introduction of living resources into the model suite, so mesozooplankton

must be modeled. The microzooplankton have no commercial value nor are they a primary food source for the finfish. They are an important prey for the mesozooplankton, however. More importantly, they can be significant predators on the phytoplankton. Omission of the microzooplankton requires a hybrid predation term on the phytoplankton in which predation by mesozooplankton is computed but predation by microzooplankton is specified. In view of the problems associated with a formulation of this sort it is easier to include microzooplankton in the model than it is to omit them. Heterotrophic bacteria are crucial components of the ecosystem. Their role in water-column respiration and in nutrient recycling is conventionally represented as first-order organic matter decay processes. These representations are adequate and, in view of the complication of modeling both bacterial biomass and activity, can be left unchanged. Any problem with omitting bacteria lies not with inadequate representation of bacterial processes but with omission of a microzooplankton food source. For the present, the omission is circumvented by allowing microzooplankton to graze directly on DOC. The predation on mesozooplankton by finfish is handled as a predation term which closes the mesozooplankton equation.

Model Carbon Cycle

Once the conceptual model has been formulated, the new state variables can be added to the previously-established model carbon cycle. The resulting cycle (Figure 2) includes: three algal groups (spring diatoms, green algae, and freshwater bloom-forming cyanobacteria); two zooplankton groups (mesozooplankton and microzooplankton); two detritus groups (labile and refractory particulate organic carbon); and dissolved organic carbon. In the absence of finfish biomass, mass is conserved by routing consumed mesozooplankton back to the detrital and dissolved organic carbon pools.

Additional Cycles

The eutrophication model also simulates cycling of nitrogen, phosphorus, silica, and dissolved oxygen. The flows of nitrogen and phosphorus through the system largely resemble the flow of carbon. Diagrams for all these cycles can be derived from inspection of the revised carbon cycle (Figure 2) and from diagrams provided elsewhere in this report.

Zooplankton Kinetics

The Algal Production Equation

Effects of zooplankton on phytoplankton are computed in the predation term of the algal production equation:

$$\frac{\delta Bx}{\delta t} = [Gx - BMx - Wsx \cdot \frac{\delta}{\delta z}] \cdot Bx - PRx \qquad \textbf{(1)}$$

in which:

Bx = biomass of algal group x (g C m^{-3})
Gx = growth rate of algal group x (d^{-1})
BMx = basal metabolic rate of algal group x (d^{-1})
WSx = settling rate of algal group x (m d^{-1})
PRx = predation on algal group x (g C m^{-3} d^{-1})
z, t = vertical (m) and temporal (d) coordinates

Zooplankton Production Equation

Each zooplankton group is represented by an identical production equation. The two groups are distinguished largely by parameter evaluation.

$$\frac{\delta Z}{\delta t} = [Gz - BMz - Mz] \cdot Z - PRz \qquad \textbf{(2)}$$

in which:

Z = zooplankton biomass (g C m^{-3})
Gz = growth rate of zooplankton group z (d^{-1})
BMz = basal metabolic rate of zooplankton group z (d^{-1})
Mz = mortality (d^{-1})
PRz = predation on zooplankton group z (g C m^{-3} d^{-1})

Growth Rate

Grazing is represented by a maximum ration formulation equivalent to the familiar Monod formulation used to represent algal nutrient uptake. Grazing is not equivalent to growth, however. Not all prey grazed is assimilated. Grazing also requires effort which results in respiration above the basic metabolic rate. The representation of growth rate which incorporates grazing, assimilation, and respiratory loss is:

$$Gz = \frac{PAz}{KHCz + PAz} \cdot RMAXz \cdot Ez \cdot (1 - RFz) \cdot f(T) \qquad \textbf{(3)}$$

in which:

PAz = prey available to zooplankton group z (g C m^{-3})
KHCz = prey density at which grazing is halved (g C m^{-3})
RMAXz = maximum ration of zooplankton group z
(g prey C g^{-1} zooplankton C d^{-1})
Ez = assimilation efficiency of zooplankton group z ($0 \leq E \leq 1$)
RFz = fraction of assimilated prey lost to respiration ($0 \leq RF \leq 1$)
f(T) = effect of temperature on grazing

Available Prey

The computation of available prey incorporates two principles:
1) A constant, between zero and unity, determines the utilization of a prey group

by a predator,

2) A threshold density exists below which prey is not utilized.

The available portion of an algal group, for example, is determined:

$$BAxz = Max(Bx - CTz, 0) \quad \textbf{(4)}$$

in which:

BAxz = The portion of algal group x available to zooplankton group z (g C m^{-3})
CTz = The threshold concentration below which prey will not be utilized by zooplankton group z (g C m^{-3})

Prey Available to Microzooplankton. Microzooplankton are conceived to graze on dissolved organic carbon (a surrogate for bacteria), three algal groups, and organic detritus. The total prey available to microzooplankton is:

$$\begin{aligned} PAsz &= UDsz \cdot DOCAsz + \sum UBsxz \cdot BAxsz \\ &+ ULsz \cdot LPOCAsz + URsz \cdot RPOCAsz \end{aligned} \quad \textbf{(5)}$$

in which:

PA = prey available to microzooplankton (g C m^{-3})
UDsz = utilization of dissolved organic carbon by microzooplankton
UBxsz = utilization of algal group x by microzooplankton
ULsz = utilization of labile particulate organic carbon by microzooplankton
URsz = utilization of refractory particulate organic carbon by microzooplankton
DOCAsz = dissolved organic carbon available to microzooplankton (g C m^{-3})
BAxsz = algal group x available to microzooplankton (g C m^{-3})
LPOCAsz = labile particulate organic carbon available to microzooplankton (g C m^{-3})
RPOCAsz = refractory particulate organic carbon available to microzooplankton (g C m^{-3})

Prey Available to Mesozooplankton. Mesozooplankton are conceived to graze on three algal groups, microzooplankton, and organic detritus. The total prey available to mesozooplankton is:

$$\begin{aligned} PAlz &= \sum UBxlz \cdot BAxlz + USZlz \cdot SZA \\ &+ ULlz \cdot LPOCAlz + URLz \cdot RPOCAlz \end{aligned} \quad \textbf{(6)}$$

in which:

SZ = microzooplankton biomass (g C m^{-3})

Definitions and notation for remaining terms largely follow those for microzooplankton.

Utilization of Each Prey Group. The fraction of the total ration removed from each prey group is determined by the fraction of each utilizable prey group relative to total utilizable prey.

Basal Metabolism

Basal metabolism of both zooplankton groups is represented as an exponentially increasing function of temperature:

$$BMz = BMREFz \cdot e^{KTBz \cdot (T - Trz)} \quad \textbf{(7)}$$

in which:

BMREFz = metabolic rate of zooplankton group z at temperature Trz (d^{-1})
T = temperature (^oC)
KTBz = effect of temperature on metabolism of zooplankton group z ($^oC^{-1}$)

Mortality

Both zooplankton groups are subject to mortality at low dissolved oxygen concentrations. The mortality term is zero until dissolved oxygen falls below a threshold (Figure 3). Thereafter, mortality increases as dissolved oxygen decreases:

$$Mz = MZEROz \cdot [1 - \frac{DOREF}{DOCRITz}] \quad \textbf{(8)}$$

in which:

Mz = mortality of zooplankton group z (d^{-1})
MZEROz = mortality at zero dissolved oxygen concentration (d^{-1})
DOCRITz = threshold below which dissolved-oxygen-induced mortality occurs (g DO m^{-3})
DOREF = dissolved oxygen concentration when DO < DOCRIT, otherwise zero (g DO m^{-3})

Predation on Zooplankton

Mesozooplankton graze on microzooplankton. In addition, grazing on mesozooplankton by organisms not represented in the model (jellyfish, finfish) is considered. Representation of predation by organisms that are not modeled is a classic problem. Our approach results in a quadratic formulation that closes the mesozooplankton system.

Assume the predators clear a specific volume of water per unit biomass. Then predation on zooplankton is the product of the clearance rate, prey abundance, and predator abundance:

$$PRlz = F \cdot LZ \cdot HTL \quad \textbf{(9)}$$

in which:

F = clearance rate (m^3 g^{-1} predator C d^{-1})
LZ = mesozooplankton biomass (g C m^{-3})
HTL = predator biomass (g C m^{-3})

In the absence of detailed data regarding the temporal and spatial predator distribution, a reasonable assumption is that predator biomass is proportional to prey biomass, HTL = $\alpha \cdot$LZ. In that case, Equation 9 can be re-written:

$$PRz = \alpha \cdot F \cdot LZ^2 \qquad \textbf{(10)}$$

Since neither α nor F are known precisely, the logical approach is to combine their product into a single unknown, PHTlz, determined during the model calibration procedure. In addition to closure, the quadratic predation term adds desirable stability to the potential oscillatory system represented by algae and zooplankton alone.

Interfacing with the Eutrophication Model

The basic principles of the zooplankton model have been outlined above. Since this chapter is the first documentation of the zooplankton model, additional details of the interfacing of the zooplankton component with the remaining model state variables are presented here.

Effect of Zooplankton on Carbon

The rate of total carbon uptake by zooplankton is the product of the maximum ration and biomass, modified by any existing food limitation:

$$Rz = \frac{PAz}{KHCz + PAz} \cdot RMAXz \cdot f(T) \qquad \textbf{(11)}$$

in which:

Rz = ration of zooplankton group z (g prey C g^{-1} zooplankton C d^{-1})

The rate at which carbon is recycled to the environment is determined by the fraction of the ration not assimilated, by the mortality, and by predation from higher trophic levels. The recycling of all zooplankton consumed by predators enforces mass conservation on the system. Mass conservation implies that zooplankton carbon permanently removed from the system due to harvest of predators is negligibly small. The carbon recycle rate is:

$$CRRATE = [(1 - Ez) \cdot Rz + Mz] \cdot Z + PRz \qquad \textbf{(12)}$$

in which:

CRRATEz = rate of carbon recycling by zooplankton group z (g C m^{-3} d^{-1})

Once the total carbon uptake and recycle are defined, the uptake and release of each carbonaceous state variable can be obtained. The uptake is determined by the ratio of utilization of a single component to total available carbon. The distribution of released carbon is determined by a set of empirical coefficients. The effect of microzooplankton on dissolved organic carbon, for example, is:

$$\frac{\delta DOC}{\delta t} = -\frac{UDsz \cdot DOCAsz}{PAsz} \cdot Rsz \cdot SZ + CRRATEsz \cdot FDOCsz \qquad \textbf{(13)}$$

in which:

FDOCsz = fraction of carbon recycled to the dissolved organic pool by microzooplankton ($0 \leq$ FDOC ≤ 1)

Effect of Zooplankton on Algae

Algae are a fraction of the total carbon uptake. No carbon is recycled to the algal pool, however. The effect of mesozooplankton on algal group 2, for example, is:

$$\frac{\delta B2}{\delta t} = -\frac{UB2lz \cdot B2Alz}{PAlz} \cdot Rlz \cdot LZ \qquad \textbf{(14)}$$

Effect of Zooplankton on Dissolved Oxygen

Zooplankton consume dissolved oxygen through the respiratory cost of assimilating food and through basal metabolism:

$$\frac{\delta DO}{\delta t} = -[Ez \cdot RFz \cdot Rz + BMz] \cdot AOCR \cdot Z \qquad \textbf{(15)}$$

in which:

Aocr = ratio of oxygen consumed to carbon metabolized (2.67 g DO g^{-1} C)

Effect of Zooplankton on Nitrogen

The computation of zooplankton effects on nutrients must account for differing composition of zooplankton and prey. An additional complication is that the model considers organic nitrogen and phosphorus to exist independently from organic carbon. In reality, these exist as organic matter composed of carbon, nitrogen, and phosphorus, among other elements. We consider that particulate organic nitrogen and phosphorus are consumed in proportion to detrital carbon.

First, evaluate the nitrogen-to-carbon ratio in the total prey consumed. For mesozooplankton, this is:

$$ANCPlz = [\sum ANCx \cdot UBxlz \cdot BxAlz + ANCsz \cdot USZlz \cdot SZAlz] / PALZ + [\frac{ULlz \cdot LPON \cdot LPOCAlz}{LPOC} + \frac{URlz \cdot RPON \cdot RPOCAlz}{RPOC}] / PAlz \quad \textbf{(16)}$$

in which:

ANCPlz = nitrogen-to-carbon ratio in prey of mesozooplankton (g N g^{-1} C)
ANCx = nitrogen-to-carbon ratio in algal group x (g N g^{-1} C)
ANCsz = nitrogen-to-carbon ratio in microzooplankton group x (g N g^{-1} C)

Additional terms follow previous definitions and notation.

All nitrogen consumed is recycled except for the amount assimilated. Additional nitrogen is recycled through respiration, mortality, and predation on zooplankton. For mesozooplankton, for example, the nitrogen recycle rate is:

$$NRRATElz = [ANCPlz - ANClz \cdot ELz \cdot (1 - RFlz)] \cdot RLz \cdot LZ + [BMlz + Mlz] \cdot ANClz \cdot LZ + PRlz \cdot ANClz \quad \textbf{(17)}$$

in which:

NRRATElz = nitrogen recycled by mesozooplankton (g N m^{-3} d^{-1})
ANClz = nitrogen-to-carbon ratio of mesozooplankton (g N g^{-1} C)

Zooplankton do not take up dissolved organic nitrogen or ammonium. Recycle of these constituents is determined by the total recycle rate and empirical distribution coefficients. Ammonium recycle by mesozooplankton, for example, is:

$$\frac{\delta NH_4}{\delta t} = NRRATElz \cdot FNH_4lz \quad \textbf{(18)}$$

in which:

FNH_4lz = fraction of nitrogen recycled to the ammonium pool by mesozooplankton ($0 \leq FNH_4lz \leq 1$)

For particulate organic nitrogen, the recycle rate is the difference between detritus consumed and recycled. The effect of mesozooplankton on labile particulate organic nitrogen, for example, is:

$$\frac{\delta LPON}{\delta t} = -\frac{ULlz \cdot LPOCAlz}{PAlz} \cdot \frac{LPON}{LPOC} \cdot Rlz \cdot LZ + NRRATElz \cdot FLPONlz \quad \textbf{(19)}$$

Effect of Zooplankton on Phosphorus

The effect of zooplankton on phosphorus is analogous to the effects described for nitrogen.

Effect of Zooplankton on Silica

Zooplankton consume silica solely through the uptake of phytoplankton. All silica consumed is recycled. Computation of the effect of zooplankton on silica requires summation of silica consumed and allocation to the two external silica pools. The effect of microzooplankton on dissolved silica, for example, is:

$$\frac{\delta SA}{\delta t} = \frac{\sum ASCx \cdot UBxsz \cdot BxAsz}{PAsz} \cdot Rsz \cdot SZ \cdot FRSAsz \quad \textbf{(20)}$$

in which:

ASCx = silica to carbon ratio of algal group x (g Si g^{-1} C)
FRSAsz = fraction of silica recycled to dissolved pool by microzooplankton
($0 \leq FRSAsz \leq 1$)

Parameter Evaluation

Parameters in the zooplankton model (Tables 1, 2) were adapted from published values, when available, and adjusted to provide improved model results. Published values were not available for a number of empirical parameters which were evaluated largely through a recursive calibration procedure. The evaluation procedure for significant parameters is detailed below.

Composition

The classic Redfield ratios for zooplankton (Redfield et al. 1963) indicate the following ratios: nitrogen-to-carbon = 0.19 g N g^{-1} C; phosphorus to carbon = 0.025 g P g^{-1} C. A summary by Parsons et al. (1984) indicates median values of 0.22 g N g^{-1} C and 0.017 g P g^{-1} C for nitrogen-to-carbon and phosphorus-to-carbon. Model composition for both zooplankton groups closely reflects these values.

Microzooplankton Ration

The microzooplankton community in the mainstem bay consists largely of rotifers and tintinnids as well as juvenile forms of mesozooplankton and other organisms (Brownlee and Jacobs 1987). A survey of specific grazing rates

(Table 3) indicates maximum rates in excess of 2 d^{-1} are observed.

The effect of temperature on grazing (Figure 4) was described with a function of the form:

$$f(t) = e^{-KTg1 \cdot (T - Topt)^2} \quad \text{when } T \le Topt$$
$$= e^{-KTg2 \cdot (T - Topt)^2} \quad \text{when } T \ge Topt \qquad \textbf{(21)}$$

in which:

T = temperature (^oC)
Topt = optimal temperature for grazing (^oC)
KTg1 = effect of temperature below optimal on grazing ($^oC^{-2}$)
KTg2 = effect of temperature above optimal on grazing ($^oC^{-2}$)

Mesozooplankton Grazing

The mesozooplankton community of the mainstem bay consists largely of three species of copepods: *Acartia tonsa*, *Eurytemora affinis*, and *Acartia hudsonica* (Brownlee and Jacobs 1987, White and Roman 1992b). Of these, an abundance of data exists for *Acartia tonsa*. Consequently, parameterization of the mesozooplankton component was based largely on this species.

Observations collected by White and Roman (1992a) provide an excellent basis for evaluation of several model parameters. The observations are based on the body weight of an adult copepod female. Ingestion, growth, and respiration were converted to carbon specific rates (Table 4) using a mass 2.6 µg C $individual^{-1}$ derived from White and Roman (1992b).

The observations indicate maximum specific ingestion rates of 2 to 3 d^{-1}. Early experiments with the model indicated the computed phytoplankton population was not sustainable with ingestion greatly in excess of 2 d^{-1}. Consequently a value of 1.75 d^{-1} was selected. The observations are for *Acartia tonsa* which predominates from May through October (White and Roman 1992b). To account for grazing by the cold-water species, a piecewise temperature function was devised that provided grazing in winter and spring in excess of observations for *Acartia* (Figure 5).

Basal Metabolism

Ikeda (1985) presented a relationship for routine metabolism:

$$Y = a \cdot c \cdot M^b \cdot d^T \qquad \textbf{(22)}$$

in which:

Y = oxygen consumption (µL O_2 $individual^{-1}$ $hour^{-1}$)
M = body mass (mg C $individual^{-1}$)
T = temperature (^oC)

a, b, c, d = empirical constants

Ikeda linearized his equation through logarithmic transformation and evaluated parameters via linear regression.

Ikeda's relationship is, no doubt, convenient for employment in terms of conventionally-measured quantities. The equation is a dimensional nightmare, however. Several pages of conversion factors eventually yield the more tractable relationship:

$$BM = \frac{0.072 \cdot e^{0.06 \cdot (T - 20)}}{M^{0.165}} \qquad \textbf{(23)}$$

in which:

BM = carbon specific metabolic rate (d^{-1})
M = body mass (mg C $individual^{-1}$)

An interesting insight is that Ikeda's original relationship indicates respiration per individual increases with body mass while the converted relationship indicates specific respiration decreases as a function of body mass (Figure 6).

Using body masses of 0.0012 mg DW and 0.008 mg DW for a rotifer and adult *Acartia* (White and Roman 1992b) and the conversion 0.4 mg C mg^{-1} DW yields the basal metabolic rates employed in the model (Tables 1, 2). The multiplier 0.06 in Equation 23 was increased to 0.069 in the model to provide a rounded, classic Q10 of 2.

Respiration Fraction and Efficiency

Data presented by White and Roman (1992a) indicates respiration accounts for 40 to 50% of total microzooplankton and phytoplankton consumed by *Acartia*. This includes both basal metabolism and the respiratory cost of feeding. Basal metabolism by Ikeda's formula (0.185 d^{-1}) is roughly half the specific respiration derived from White and Roman's data (Table 4). These proportions indicate the respiratory fraction is the remaining half of specific respiration or 20 to 25% of prey consumed. We found a lower fraction, 7% of prey consumed, provided reasonable results when employed in the mesozooplankton computations. A higher value, 50% of prey consumed, was employed for microzooplankton to reflect the effect of body size on respiration.

The same observations indicate growth and respiration account for 87 to 95% of total ingestion. Roughly 10% of total ingestion is unaccounted for, indicating efficiency is roughly 90%. Modeled efficiencies are only one third of that value, however. While the efficiency derived from observations seems high (White and Roman assume 80%), the model values are unrealistically low. Reduced efficiencies were initially assigned to the model based on need. Efficiencies of 80 to 90% produced wide oscillations in computed populations

and resulted in collapse of the phytoplankton population. Lower efficiencies resulted in damped oscillations and more stable communities.

Later insights indicated why lower efficiencies are appropriate. In the model, adult zooplankton instantaneously reproduce adult zooplankton. In reality, reproduction is in the form of eggs. Eggs hatch into juvenile forms that eventually mature into adults. The true growth process installs temporal lags in the system and reduces efficiency as eggs and juveniles are lost to predation and other processes. While the temporal lags are difficult to introduce into the present model, the losses that occur to eggs and juveniles are simulated though employment of relatively low efficiencies.

Additional Parameters

Selection of the dissolved oxygen threshold for mortality was guided by the observation that concentrations below 1 gm DO m^{-3} result in reduced survival of copepod adults and inhibited hatching of *Acartia tonsa* eggs (Roman et al. 1993).

Sellner et al. (1993) noted neither rotifers nor copepods grazed heavily on *Microcystis*. Consequently, utilization of Group 1 algae, which represent cyanobacteria in the tidal fresh Potomac River, was set to zero. White and Roman's (1992a) observations indicate consumption of microzooplankton by mesozooplankton is comparable to consumption of phytoplankton. Consequently utilization of microzooplankton was set to unity.

Selection of half-saturation and threshold concentrations for mesozooplankton was guided by interpretation of numerous studies (Table 5). Smaller concentrations were employed for microzooplankton to reflect their smaller body size.

Observations

Zooplankton biomass was monitored at 27 stations throughout the mainstem and tributaries (Figure 7). Mesozooplankton were sampled monthly, using a 202 μm net towed obliquely from bottom to surface, and quantified as dry weight. For comparison with the model, mesozooplankton biomass was converted from dry weight to carbon using the ratio 0.4 gm C gm^{-1} DW. Microzooplankton were sampled monthly, in the Maryland portion of the bay only, using a 44 μm net. Five samples from above the pycnocline were combined into "surface mixed layer" composites. Five samples from below the pycnocline were combined into "bottom mixed layer" composites. The investigators computed total biomass, as carbon, from species counts using standard biomass for individuals of each species. The data base, extending from mid-1984 through 1994, was provided by the Chesapeake Bay Program Office (Maryland) and by investigators at Old Dominion University (Virginia).

Model Results

Model Time Series

Model results were compared to observed time series at all stations for which data were available. Comparisons were consistent with sampling procedure. Mesozooplankton were sampled in oblique vertical casts that provided a vertically-integrated sample. Modeled mesozooplankton was vertically averaged for comparison with the observations. Microzooplankton observations were composite samples representing "above pycnocline" and "below pycnocline" concentrations. Model results from individual cells were combined into above- and below-pycnocline values. The observed pycnocline depth varies spatially and temporally and is not always distinct. For comparison with the observations, the model pycnocline was assumed to occur at a consistent depth of 6.7 m (upper four model layers). In the event the total depth was less than 6.7 m, the entire model water column was combined into the above pycnocline value. A sampling of results is presented here.

The time series of observed and modeled zooplankton are difficult to interpret, primarily due to the large variance inherent in the observations. Some basic observations are possible, however. Within the mainstem of the bay, observed peak microzooplankton abundance is roughly twice as high above pycnocline than below pycnocline. The model demonstrates lesser difference above and below pycnocline and is closer to the observed below-pycnocline values (Figures 8,9). Although a few extreme observations exceed modeled values, the model reproduces the preponderance of mesozooplankton observations in the mainstem bay (Figure 10).

Effect of Dissolved Oxygen

The model includes a mortality factor to account for the impact of anoxia on zooplankton (Equation 8). The vertical tows used to sample mesozooplankton do not allow distinction of surface and bottom populations in regions where anoxia occurs. The model computes substantial differences between surface and bottom populations in the presence of anoxia. At a mid-bay station, computed surface and bottom populations of mesozooplankton are nearly identical from January thorough April (Figure 11). In April the populations diverge and mesozooplankton at the bottom are nearly extinct from June through August. In September, the bottom population recovers and is equivalent to the surface by November. The mesozooplankton time series at bottom is consistent with the time series of computed dissolved oxygen (Figure 12). The divergence between surface and bottom populations begins when computed bottom dissolved oxygen plunges towards zero. Mesozooplankton at the bottom remain at low levels until the autumn turnover period and gradually recover to surface levels throughout the autumn.

Cumulative Distributions

Little or no correspondence exists between individual observations and model computations. In view of the large, random variance in the observations, lack of one-to-one correspondence is expected. An alternate, more informative view can be obtained by comparing the cumulative distributions of observed and computed zooplankton. The computed distributions are based on model computations corresponding to sample locations and days. The computed

distributions do not represent the population of computations.

Within the mainstem bay, the observed microzooplankton exceed computed by 50% to 100% throughout most of the distribution (Figure 13). Agreement between computed and observed mesozooplankton is excellent throughout the distribution in the mainstem bay (Figure 14).

Recommendations for Improvement

The present model represents zooplankton biomass within 50% to 100% of observed values, as determined by comparisons of cumulative distributions. Discrepancies between observations and model certainly indicate shortcomings in the model. A large portion of the discrepancies, however, must be attributed to observational methodology and to the variance inherent in the populations. A high degree of accuracy is unlikely to be obtained but more realism and, potentially, more accuracy can be added to the model. Suggestions for improvement range from parameter re-evaluation through complete model reformulation.

The computed time series of both microzooplankton and mesozooplankton exhibit semi-annual cycles with two peaks per year (Figures 8, 10). Analysis of model results from the Virginia Tributary Refinements phase (Cerco and Meyers 2000) indicated the mid-year dip in microzooplankton was due to grazing by mesozooplankton. The dip in mesozooplankton was attributed to anoxia in the mainstem bay. An alternate explanation for the dips in both populations may lie with the temperature dependence of the grazing and respiration functions. Grazing in both populations peaks at roughly 25 ^{o}C (Figures 4, 5) while metabolism increases indefinitely as a function of temperature (Equation 7). Consequently, at high mid-summer temperatures, an excess of metabolism over grazing may cause a decline in computed zooplankton. The effects of temperature on grazing and respiration should be reviewed and the cause of the mid-year population dips re-established. If the dips are due to the temperature functions, re-evaluation of the parameters that describe temperature effects on grazing may be appropriate.

Another potential improvement is to add a second mesozooplankton group. One group would represent the winter-spring population; the second group would represent the summer population. No doubt, these two populations exist and can be differentiated. The second group can be readily included and adds realism to the model. The potential quantitative improvement in model computations cannot be foreseen.

The final improvement is the most difficult. Add age structure to the mesozooplankton model. As previously noted, adults in the present model instantaneously reproduce adults. In the most realistic model, adults would produce eggs. Eggs would hatch into larvae, mature into juveniles and, later, into adults. A model of this sort offers the highest probability of success in representing the time series of observed mesozooplankton. A multi-stage population model requires tremendous resources in programming, calibration, and execution. The additional effort is likely not worthwhile in the present multi-

purpose model. The improvement is highly recommended if the present model is employed in an application that focuses largely on zooplankton.

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Table 1
Parameters in Microzooplankton Model

Parameter	Description	Value	Units
ANCsz	nitrogen to carbon ratio	0.2	g N g^{-1} C
AOCRsz	ratio of oxygen consumed to carbon metabolized	2.67	g DO g^{-1} C
APCsz	phosphorus to carbon ratio	0.02	g P g^{-1} C
BMREFsz	basal metabolism at reference temperature	0.254	d^{-1}
CTsz	carbon threshold for grazing	0.01	g C m^{-3}
DOCRITsz	concentration below which dissolved oxygen mortality occurs	2.0	g DO m^{-3}
Esz	assimilation efficiency	0.3	$0 \leq E \leq 1$
FDOCsz	fraction of carbon recycled to dissolved organic pool	0.25	$0 \leq FDOC \leq 1$
FDONsz	fraction of nitrogen recycled to dissolved organic pool	0.20	$0 \leq FDON \leq 1$
FDOPsz	fraction of phosphorus recycled to dissolved organic pool	0.40	$0 \leq FDOP \leq 1$
FLPOCsz	fraction of carbon recycled to labile particulate organic pool	0.50	$0 \leq FLPOC \leq 1$
FLPONsz	fraction of nitrogen recycled to labile particulate organic pool	0.25	$0 \leq FLPON \leq 1$
FLPOPsz	fraction of phosphorus recycled to labile particulate organic pool	0.07	$0 \leq FLPOP \leq 1$
FNH4sz	fraction of nitrogen recycled to dissolved inorganic pool	0.40	$0 \leq FNH4 \leq 1$
FPO4sz	fraction of phosphorus recycled to dissolved inorganic pool	0.50	$0 \leq FPO4 \leq 1$
FRPOCsz	fraction of carbon recycled to refractory particulate organic pool	0.25	$0 \leq FRPOC \leq 1$
FRPONsz	fraction of nitrogen recycled to refractory particulate organic pool	0.15	$0 \leq FRPON \leq 1$
FRPOPsz	fraction of phosphorus recycled to refractory particulate organic pool	0.03	$0 \leq FRPOP \leq 1$
FRSAsz	fraction of silica recycled to dissolved pool	0.55	$0 \leq FRSA \leq 1$
KHCsz	prey density at which grazing is halved	0.05	g C m^{-3}
KTBGsz	effect of temperature on basal metabolism	0.069	$^oC^{-1}$
KTGsz1	effect of sub-optimal temperature on grazing	0.0035	$^oC^{-2}$
KTGsz2	effect of super-optimal temperature on grazing	0.025	$^oC^{-2}$
MZEROsz	mortality at zero dissolved oxygen concentration	4.0	d^{-1}
RMAXsz	maximum ration	2.25	g prey C g^{-1} zooplankton C d^{-1}
RFsz	fraction of assimilated prey lost to respiration	0.5	$0 \leq RF \leq 1$
TMsz	optimal temperature for grazing	25	^oC

TRsz	reference temperature for basal metabolism	20	^{o}C
UB1sz	utilization of algal group 1	0.0	$0 \leq UB1sz \leq 1$
UB2sz	utilization of algal group 2	1.0	$0 \leq UB2sz \leq 1$
UB3sz	utilization of algal group 1	1.0	$0 \leq UB3sz \leq 1$
UDsz	utilization of dissolved organic carbon	0.1	$0 \leq UDsz \leq 1$
ULsz	utilization of labile particulate organic carbon	0.1	$0 \leq ULsz \leq 1$
URsz	utilization of refractory particulate organic carbon	0.1	$0 \leq URsz \leq 1$

Table 2
Parameters in Mesozooplankton Model

Parameter	Description	Value	Units
ANClz	nitrogen to carbon ratio	0.2	g N g^{-1} C
AOCRlz	ratio of oxygen consumed to carbon metabolized	2.67	g DO g^{-1} C
APClz	phosphorus to carbon ratio	0.02	g P g^{-1} C
BMREFlz	basal metabolism at reference temperature	0.186	d^{-1}
CTlz	carbon threshold for grazing	0.05	g C m^{-3}
DOCRITlz	concentration below which dissolved oxygen mortality occurs	2.0	g DO m^{-3}
Elz	assimilation efficiency	0.30	$0 \leq E \leq 1$
FDOClz	fraction of carbon recycled to dissolved organic pool	0.25	$0 \leq$ FDOC ≤ 1
FDONlz	fraction of nitrogen recycled to dissolved organic pool	0.20	$0 \leq$ FDON ≤ 1
FDOPlz	fraction of phosphorus recycled to dissolved organic pool	0.40	$0 \leq$ FDOP ≤ 1
FLPOClz	fraction of carbon recycled to labile particulate organic pool	0.50	$0 \leq$ FLPOC ≤ 1
FLPONlz	fraction of nitrogen recycled to labile particulate organic pool	0.25	$0 \leq$ FLPON ≤ 1
FLPOPlz	fraction of phosphorus recycled to labile particulate organic pool	0.07	$0 \leq$ FLPOP ≤ 1
FNH4lz	fraction of nitrogen recycled to dissolved inorganic pool	0.40	$0 \leq$ FNH4 ≤ 1
FPO4lz	fraction of phosphorus recycled to dissolved inorganic pool	0.50	$0 \leq$ FPO4 ≤ 1
FRPOClz	fraction of carbon recycled to refractory particulate organic pool	0.25	$0 \leq$ FRPOC ≤ 1
FRPONlz	fraction of nitrogen recycled to refractory particulate organic pool	0.15	$0 \leq$ FRPON ≤ 1
FRPOPlz	fraction of phosphorus recycled to refractory particulate organic pool	0.03	$0 \leq$ FRPOP ≤ 1
FRSAlz	fraction of silica recycled to dissolved pool	0.55	$0 \leq$ FRSA ≤ 1
KHClz	prey density at which grazing is halved	0.175	g C m^{-3}
KTBGlz	effect of temperature on basal metabolism	0.069	$^oC^{-1}$
KTGlz1	effect of sub-optimal temperature on grazing	0.008	$^oC^{-2}$
KTglz2	effect of super-optimal temperature on grazing	0.03	$^oC^{-2}$
KTPRlz	effect of temperature on predation by higher trophic levels	0.069	$^oC^{-1}$
MZEROlz	mortality at zero dissolved oxygen concentration	4.0	d^{-1}
PHTlz	predation by higher trophic levels	2.0	m^3 g^{-1} C d^{-1}
RMAXlz	maximum ration	1.75	g prey C g^{-1} zooplankton C d^{-1}

RFlz	fraction of assimilated prey lost to respiration	0.07	$0 \leq RF \leq 1$
TMlz	optimal temperature for grazing	25	^{o}C
TPRlz	reference temperature for predation by higher trophic levels	20	^{o}C
TRlz	reference temperature for basal metabolism	20	^{o}C
UB1sz	utilization of algal group 1	0.0	$0 \leq UB1sz \leq 1$
UB2sz	utilization of algal group 2	1.0	$0 \leq UB2sz \leq 1$
UB3sz	utilization of algal group 1	1.0	$0 \leq UB3sz \leq 1$
ULsz	utilization of labile particulate organic carbon	0.1	$0 \leq ULsz \leq 1$
URsz	utilization of refractory particulate organic carbon	0.1	$0 \leq URsz \leq 1$
USZlz	utilization of microzooplankton	1.0	$0 \leq USZlz \leq 1$

Table 3
Microzooplankton Specific Ingestion

Temperature (oC)	Ingestion (1/d)	Organism	Source
5.5	0.79	A. hudsonica nauplii	White and Roman, 1992b
9.5	0.37	rotifer	White and Roman, 1992b
18.5	0.54	ciliate	Dagg, 1995
20.5	2.8	A. tonsa nauplii	White and Roman, 1992b
20.5	0.32	ciliate	Dagg, 1995
30.1	1.08	ciliate	Dagg, 1995
30.3	0.84	ciliate	Dagg, 1995
30.4	2.11	ciliate	Dagg, 1995
30.4	1.38	ciliate	Dagg, 1995

Table 4
Ingestion, Growth, and Respiration for an Adult Female Acartia Tonsa (after White and Roman 1992a)

Temp (°C)	Growth (µg C/ female/d)	Phyto Ingest (µg C/ female/d)	MicroZ Ingest (µg C/ female/d)	Respiration (µg C/ female/ d)	Growth (1/d)	Phyto Ingest (1/d)	Respiration (1/d)
16.8	1.16	0.69		0.7	0.45	0.27	0.27
23.5	0.67	2.26		0.98	0.26	0.87	0.38
26.9	2.07	3.35		0.9	0.80	1.29	0.35
27.6	0.68	6.86		0.93	0.26	2.64	0.36
17.1	0.64	0.28	1.15	0.72	0.25	0.11	0.28
18.7	1.58	0.99		0.8	0.61	0.38	0.31
19.3	1.89	0.01		0.81	0.73	0.00	0.31
20	1.91	9.2		0.82	0.73	3.54	0.32
27.2	1.06	4.71		1.12	0.41	1.81	0.43
29.4	1.21	2.4	0.36	1.2	0.47	0.92	0.46
26	2.01	4.69		0.98	0.77	1.80	0.38
24.2	2.3	5.82		0.89	0.88	2.24	0.34
15.8	0.71	0.68		0.64	0.27	0.26	0.25

Table 5
Mesozooplankton Threshold and Half Saturation Concentrations

mg C / L	Comment	Source
0.01	for growth	Kiorboe and Nielson (1994)
0.7	egg production	Durbin et al. (1983)
0.05	clearance rates decrease	Paffenhofer and Stearns (1988)
0.175	A. nauplii growth	Berggreen et al. (1988)
0.2	ingestion	Kiorboe et al. (1985)

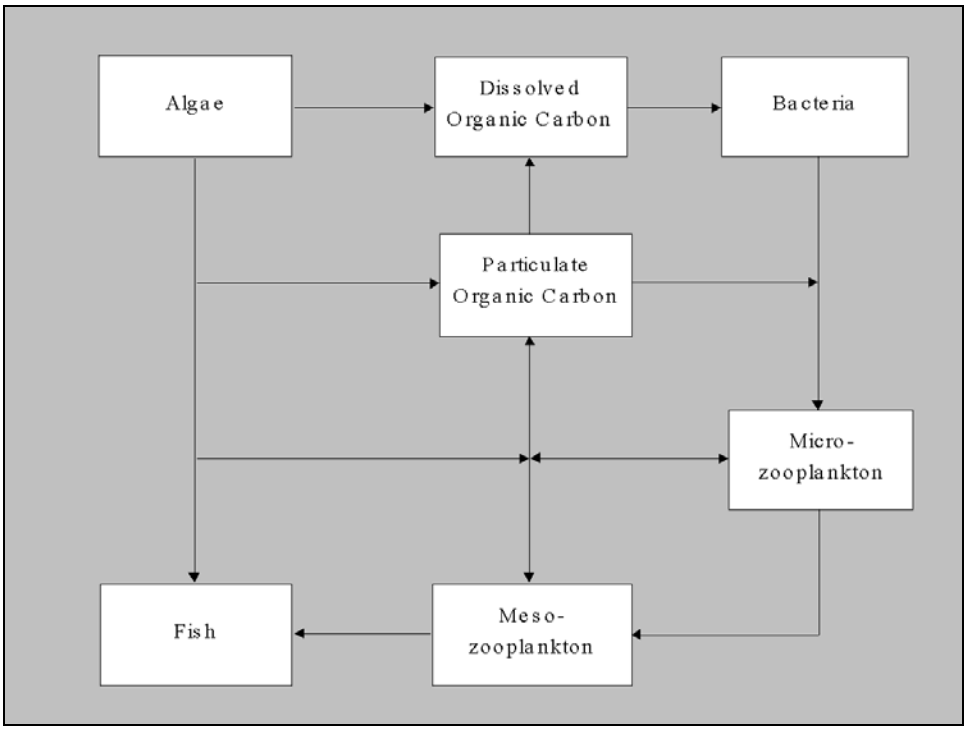

Figure 1. The conceptual carbon cycle

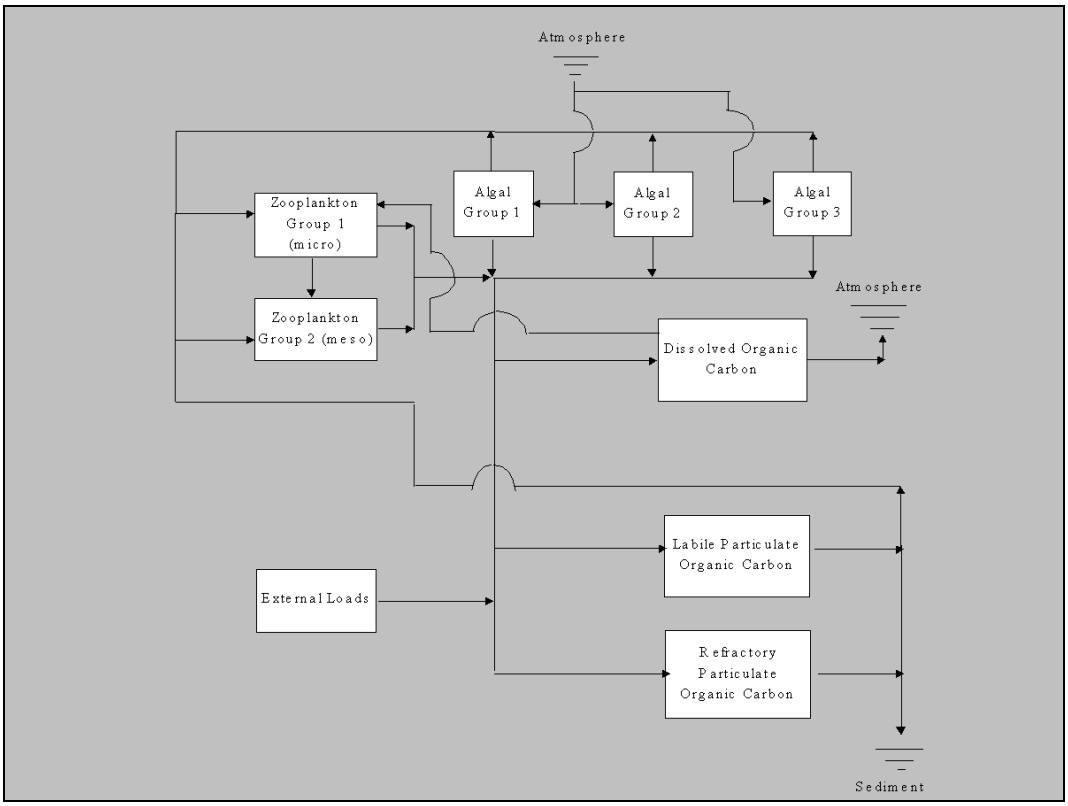

Figure 2. The model carbon cycle

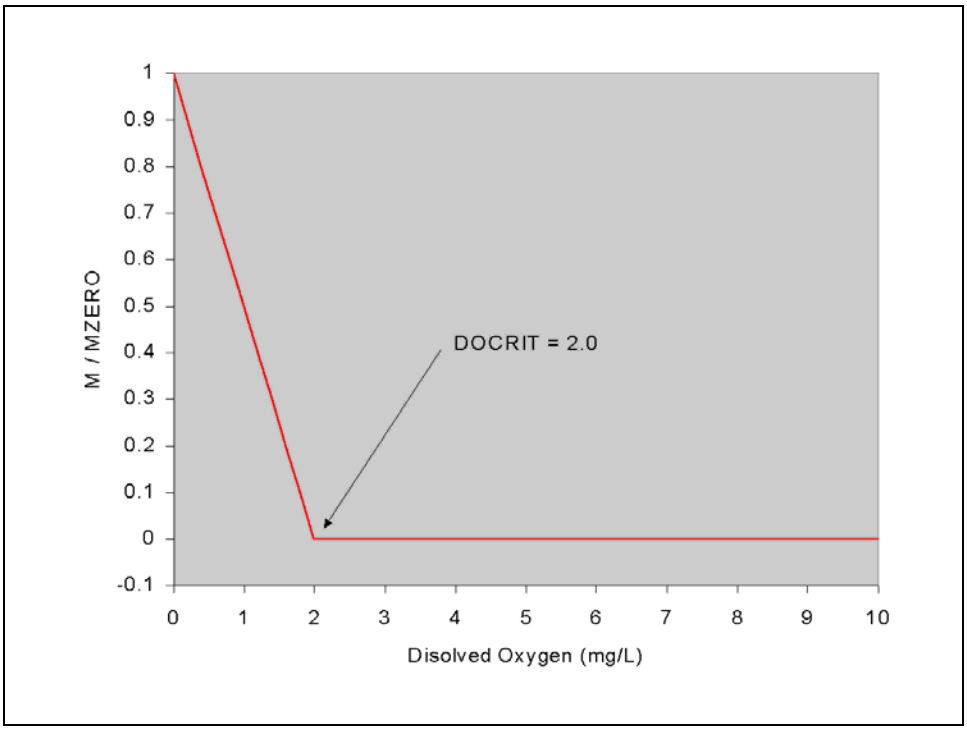

Figure 3. Dissolved oxygen mortality function

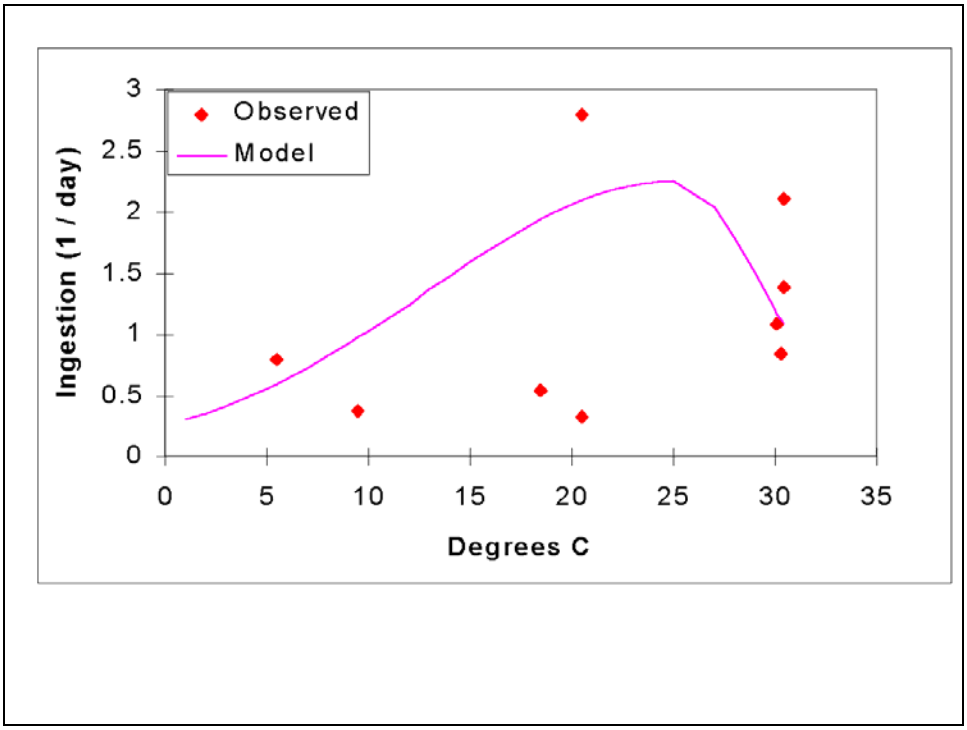

Figure 4. Effect of temperature on microzooplankton grazing

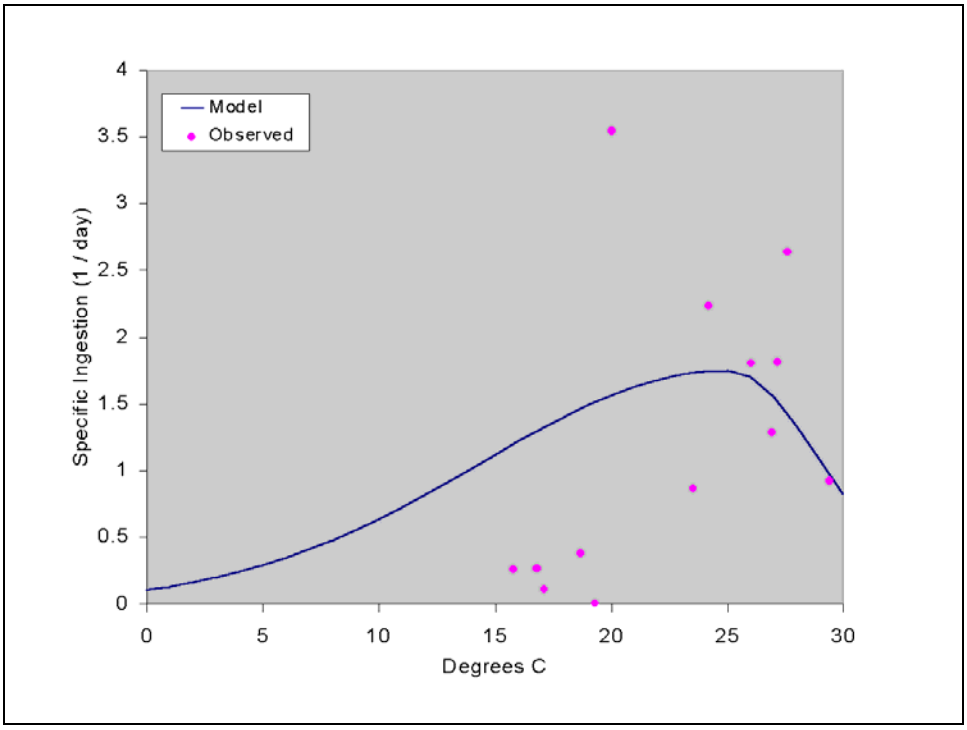

Figure 5. Effect of temperature on mesozooplankton grazing

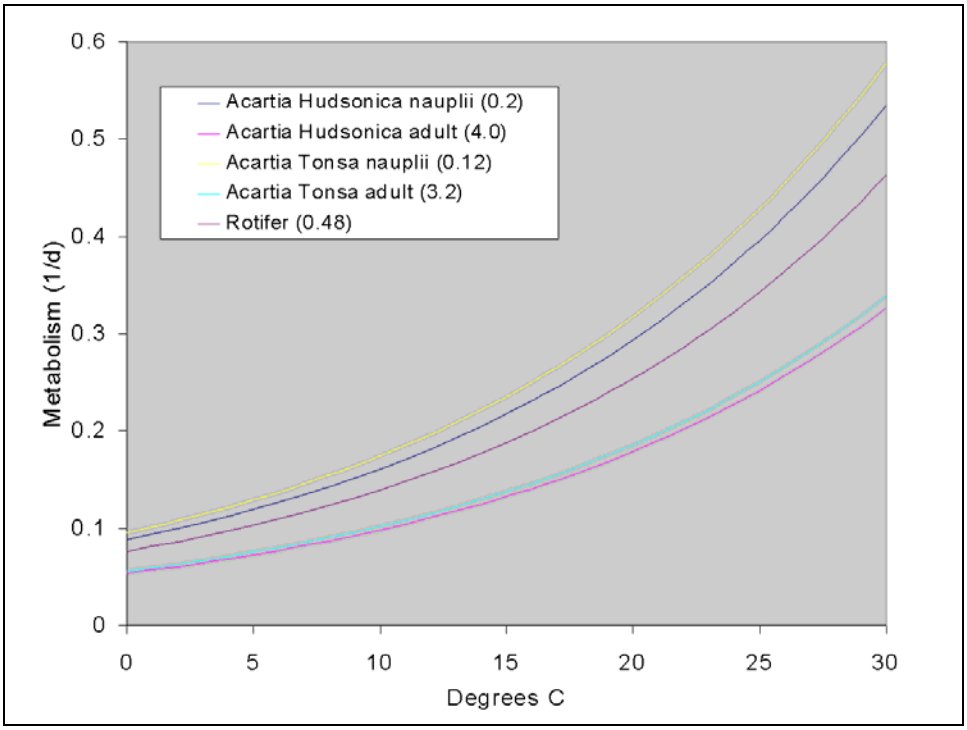

Figure 6. Effect of body size (µg C) and temperature on specific, basal metabolism. Size from White and Roman (1992b).

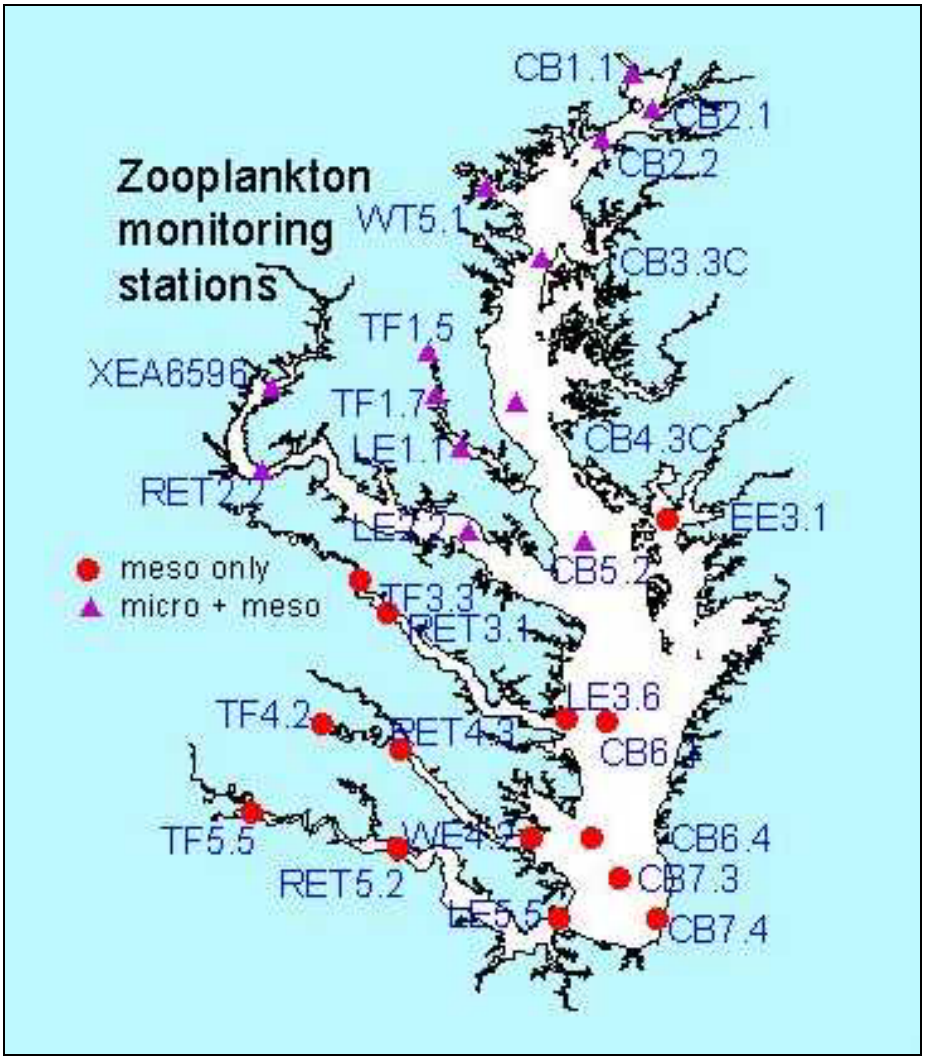

Figure 7. Zooplankton sampling stations.

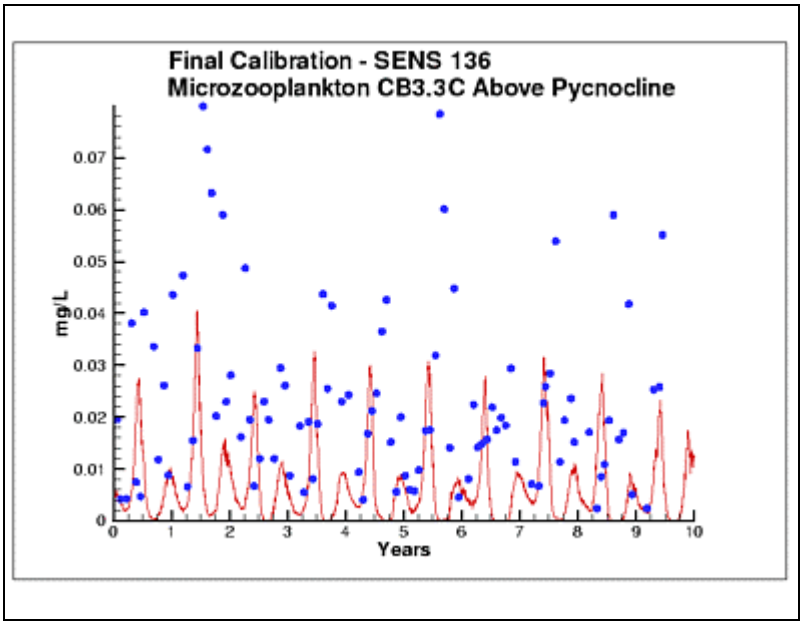

Figure 8. Time series of computed and observed microzooplankton, above pycnocline, at Station CB3.3C in the mainstem Chesapeake Bay.

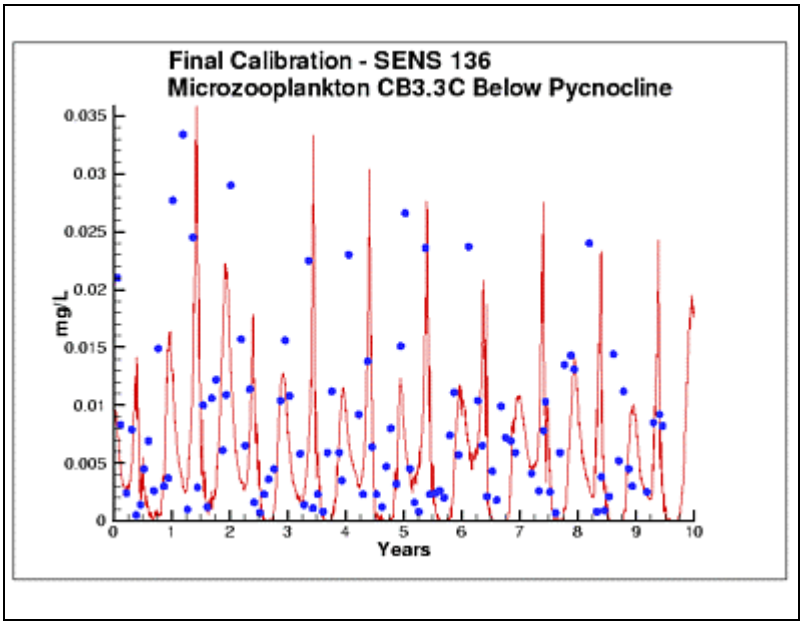

Figure 9. Time series of computed and observed microzooplankton, below pycnocline, at Station CB3.3C in the mainstem Chesapeake Bay.

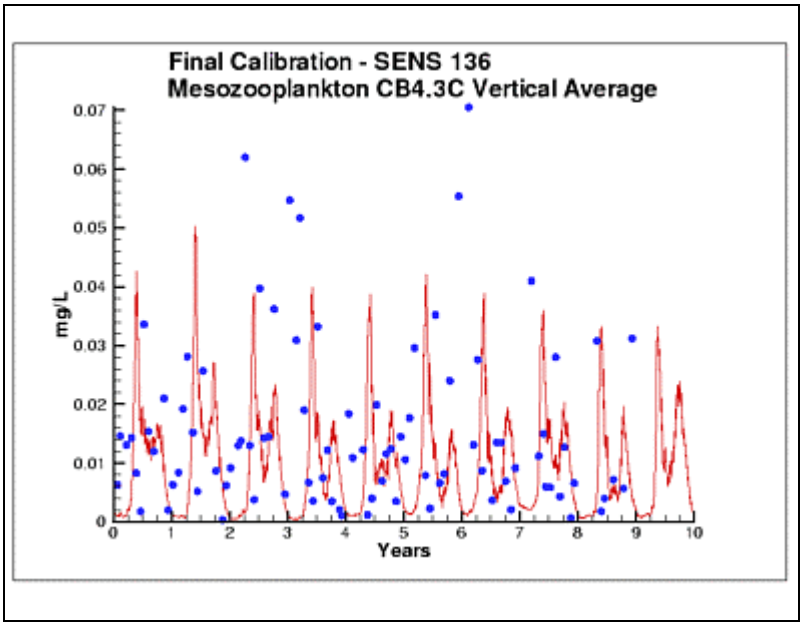

Figure 10. Time series of computed and observed mesozooplankton at Station CB4.3C in the mainstem Chesapeake Bay.

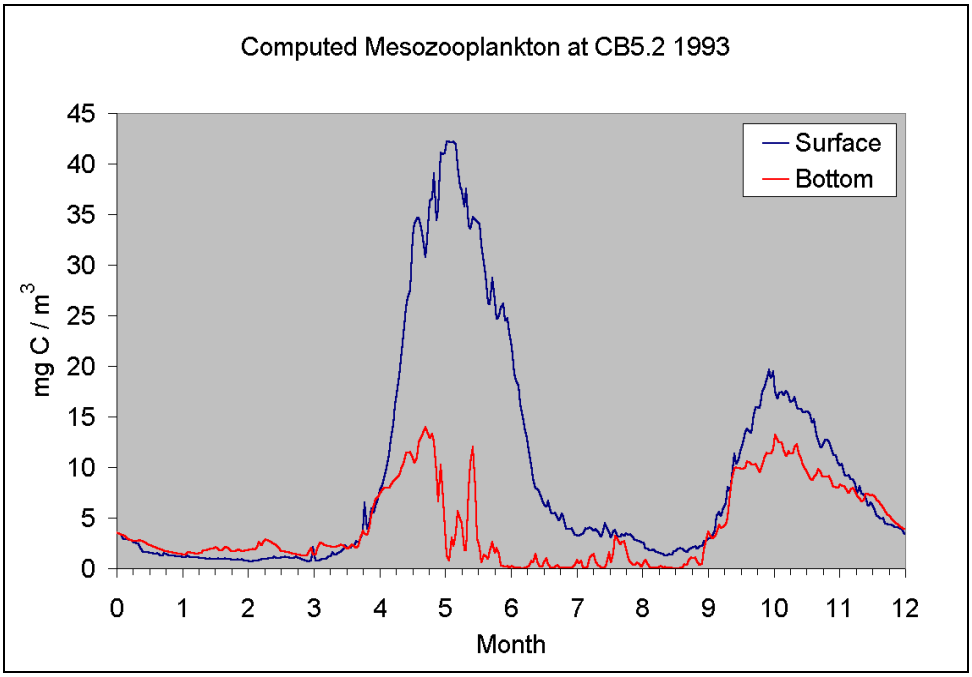

Figure 11. Time series of computed mesozooplankton, surface and bottom, at Station CB5.2 in the mainstem Chesapeake Bay for 1993.

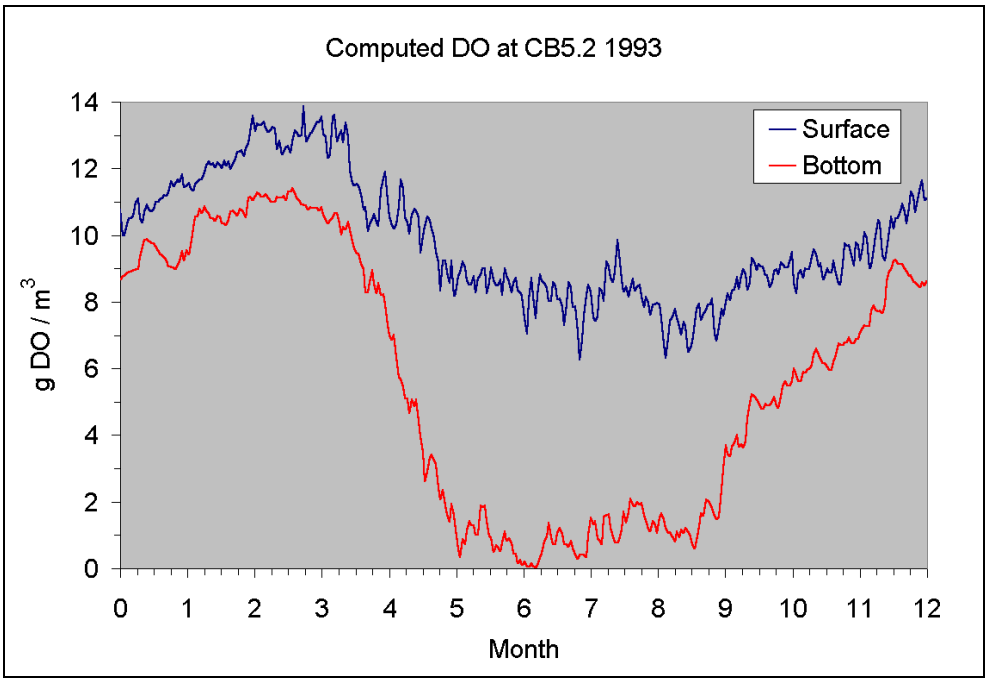

Figure 12. Time series of computed dissolved oxygen, surface and bottom, at Station CB5.2 in the mainstem Chesapeake Bay for 1993.

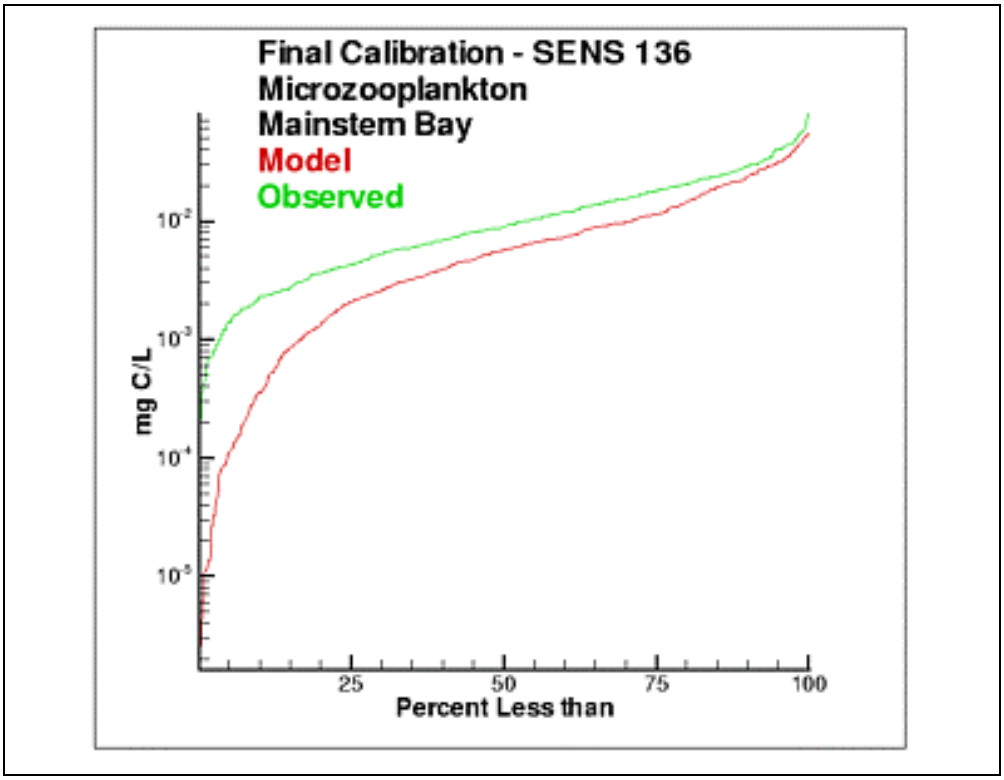

Figure 13. Cumulative distribution of computed and observed microzooplankton in the mainstem bay.

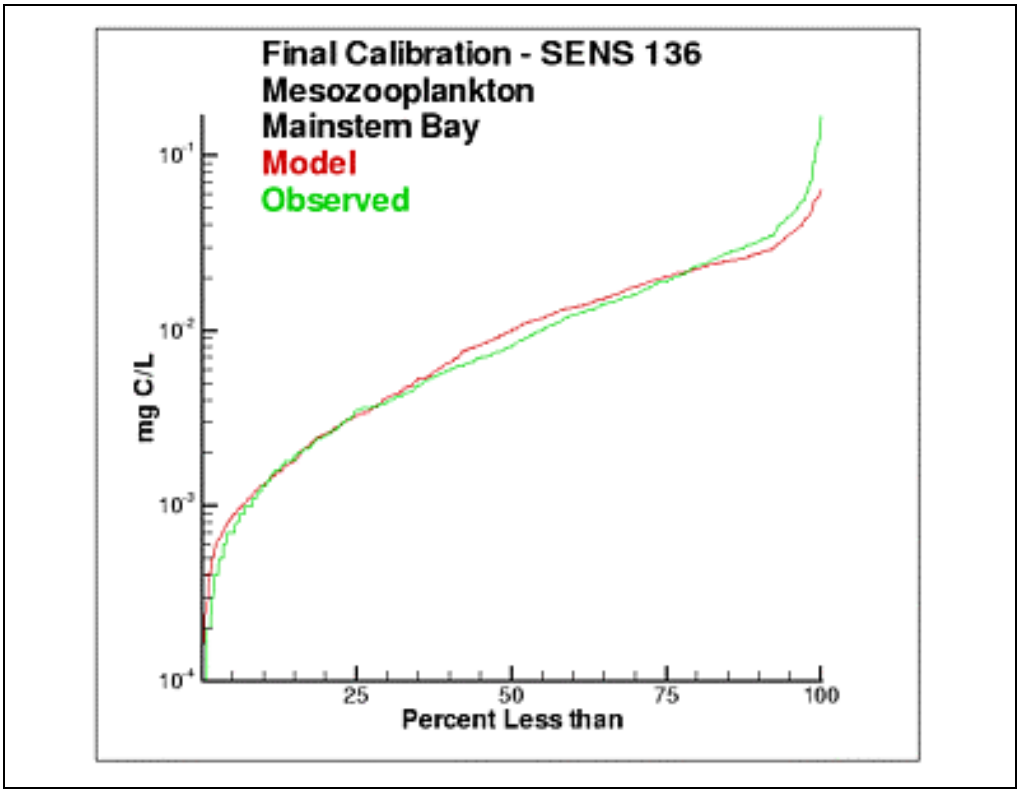

Figure 14. Cumulative distribution of computed and observed mesozooplankton in the mainstem bay (CB2-CB7)

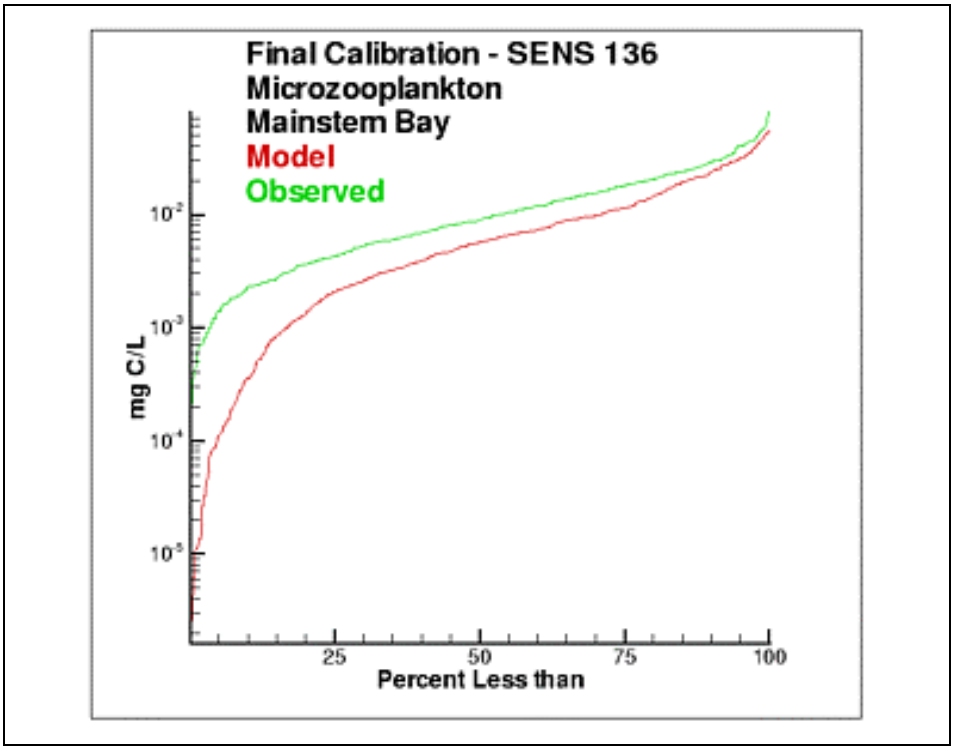

Figure 13. Cumulative distribution of computed and observed microzooplankton in the mainstem bay (CB2-CB5)

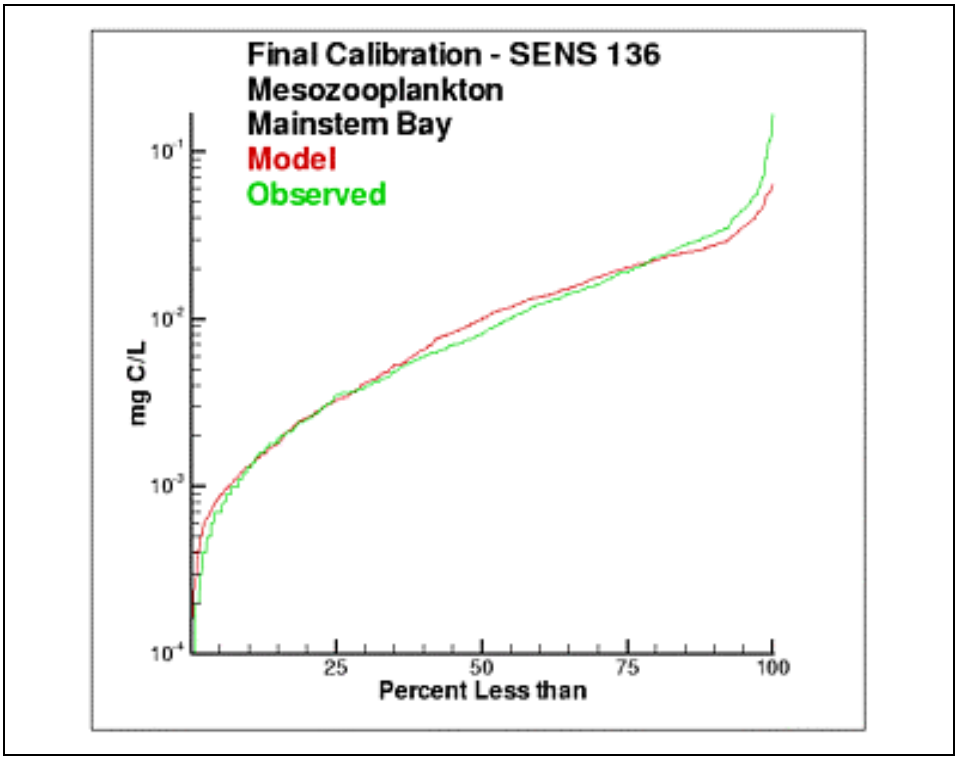

Figure 14. Cumulative distribution of computed and observed mesozooplankton in the mainstem bay (CB2-CB7)

The Zooplankton Input File

The Zooplankton Input File contains five sections. These are a title, a section of spatially-uniform parameters, a section of spatially-varying parameters, a section of temporally-varying parameters, and a section of temperature-dependent rates.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe zooplankton input deck

Six title lines are required to describe the zooplankton input deck. These are not read as variables but are skipped by a FORMAT statement.

Example

```
Map calibration zooplankton growth rates onto 12,920-cell grid.
Set ocean rates to zero.  Rest same as wqm_zoo.sens31.  Feb 2, 2001
Modify splits of detritus.  Put more into NH4, LPON, less into PON
Increase efficiency of mesozooplankton from 0.25 to 0.30
Increase efficiency of microzooplankton from 0.25 to 0.30
March 9, 2001
```

Spatially-Uniform Parameters

Each group of the spatially-uniform parameters follows the same convention – a blank line, a parameter list, and a line of parameter values. The format for each group is (//(8X,9F8.0)).

Field	Name	Value	Description
1	CTSZ	Real	Microzooplankton carbon threshold for grazing (g C m^{-3})
2	KHCSZ	Real	Prey density at which microzooplankton grazing is halved (g C m^{-3})
3	DOCRTSZ	Real	Concentration below which microzooplankton mortality occurs (g DO m^{-3})
4	MZEROSZ	Real	Microzooplankton mortality at zero dissolved oxygen (d^{-1})
1	ANCSZ	Real	Microzooplankton nitrogen-to-carbon ratio (g N g^{-1} C)

2	APCSZ	Real	Microzooplankton phosphorus-to-carbon ratio (g N g^{-1} C)
3	AOCRSZ	Real	Microzooplankton ratio of oxygen consumed to carbon metabolized (g DO g^{-1} C)
1	UBCSZ	Real	Microzooplankton utilization of algal group 1 ($0 \leq$ UBCSZ ≤ 1)
2	UBDSZ	Real	Microzooplankton utilization of algal group 2 ($0 \leq$ UBDSZ ≤ 1)
3	UBGSZ	Real	Microzooplankton utilization of algal group 3 ($0 \leq$ UBGSZ ≤ 1)
4	UDSZ	Real	Microzooplankton utilization of dissolved organic carbon ($0 \leq$ UDSZ ≤ 1)
5	ULSZ	Real	Microzooplankton utilization of labile particulate organic carbon ($0 \leq$ UDSZ ≤ 1)
6	URSZ	Real	Microzooplankton utilization of refractory particulate organic carbon ($0 \leq$ UDSZ ≤ 1)
1	TMSZ	Real	Optimal temperature for microzooplankton grazing (^oC)
2	KTGSZ1	Real	Effect of sub-optimal temperature on microzooplankton grazing ($^oC^{-2}$)
3	KTGSZ2	Real	Effect of super-optimal temperature on microzooplankton grazing ($^oC^{-2}$)
4	TRSZ	Real	Reference temperature for microzooplankton basal metabolism (^oC)
5	KTBSZ	Real	Effect of temperature on microzooplankton basal metabolism ($^oC^{-1}$)
6	TPRSZ	Real	Reference temperature for non-specific predation on microzooplankton (^oC)
7	KTPRSZ	Real	Effect of temperature on non-specific predation on microzooplankton ($^oC^{-1}$)
1	FDOCSZ	Real	Fraction of microzooplankton carbon released to dissolved organic pool ($0 \leq$ FDOCSZ ≤ 1)
2	FLPOCSZ	Real	Fraction of microzooplankton carbon released to labile particulate pool ($0 \leq$ FLPOCSZ ≤ 1)
3	FRPOCSZ	Real	Fraction of microzooplankton carbon released to refractory particulate pool ($0 \leq$ FRPOCSZ ≤ 1)
1	FNH4SZ	Real	Fraction of microzooplankton nitrogen released as ammonium ($0 \leq$ FNH4SZ ≤ 1)
2	FDONSZ	Real	Fraction of microzooplankton nitrogen released to dissolved organic pool ($0 \leq$ FDONSZ ≤ 1)

3	FLPONSZ	Real	Fraction of microzooplankton nitrogen released to labile particulate pool ($0 \leq$ FLPONSZ ≤ 1)
4	FRPONSZ	Real	Fraction of microzooplankton nitrogen released to refractory particulate pool ($0 \leq$ FRPONSZ ≤ 1)
1	FPO4SZ	Real	Fraction of microzooplankton phosphorus released as phosphate ($0 \leq$ FPO4SZ ≤ 1)
2	FDOPSZ	Real	Fraction of microzooplankton phosphorus released to dissolved organic pool ($0 \leq$ FDOPSZ ≤ 1)
3	FLPOPSZ	Real	Fraction of microzooplankton phosphorus released to labile particulate pool ($0 \leq$ FDOPSZ ≤ 1)
4	FRPOPSZ	Real	Fraction of microzooplankton phosphorus released to refractory particulate pool ($0 \leq$ FDOPSZ ≤ 1)
1	FRSASZ	Real	Fraction of silica released by microzooplankton to dissolved pool ($0 \leq$ FRSASZ ≤ 1)
1	CTLZ	Real	Mesozooplankton carbon threshold for grazing (g C m^{-3})
2	KHCLZ	Real	Prey density at which mesozooplankton grazing is halved (g C m^{-3})
3	DOCRTLZ	Real	Concentration below which mesozooplankton mortality occurs (g DO m^{-3})
4	MZEROLZ	Real	Mesozooplankton mortality at zero dissolved oxygen (d^{-1})
1	ANCLZ	Real	Mesozooplankton nitrogen-to-carbon ratio (g N g^{-1} C)
2	APCLZ	Real	Mesozooplankton phosphorus-to-carbon ratio (g N g^{-1} C)
3	AOCRLZ	Real	Mesozooplankton ratio of oxygen consumed to carbon metabolized (g DO g^{-1} C)
1	UBCLZ	Real	Mesozooplankton utilization of algal group 1 ($0 \leq$ UBCLZ ≤ 1)
2	UBDLZ	Real	Mesozooplankton utilization of algal group 2 ($0 \leq$ UBDLZ ≤ 1)
3	UBGLZ	Real	Mesozooplankton utilization of algal group 3 ($0 \leq$ UBGLZ ≤ 1)
4	USZLZ	Real	Mesozooplankton utilization of microzooplankton ($0 \leq$ USZLZ ≤ 1)
5	ULLZ	Real	Mesozooplankton utilization of labile particulate organic carbon ($0 \leq$ UDLZ ≤ 1)

6	URLZ	Real	Mesozooplankton utilization of refractory particulate organic carbon ($0 \leq$ UDLZ ≤ 1)
1	TMLZ	Real	Optimal temperature for mesozooplankton grazing (^oC)
2	KTGLZ1	Real	Effect of sub-optimal temperature on mesozooplankton grazing ($^oC^{-2}$)
3	KTGLZ2	Real	Effect of super-optimal temperature on mesozooplankton grazing ($^oC^{-2}$)
4	TRLZ	Real	Reference temperature for mesozooplankton basal metabolism (^oC)
5	KTBLZ	Real	Effect of temperature on mesozooplankton basal metabolism ($^oC^{-1}$)
6	TPRLZ	Real	Reference temperature for predation on mesozooplankton (^oC)
7	KTPRLZ	Real	Effect of temperature on predation on mesozooplankton ($^oC^{-1}$)
1	FDOCLZ	Real	Fraction of mesozooplankton carbon released to dissolved organic pool ($0 \leq$ FDOCLZ ≤ 1)
2	FLPOCLZ	Real	Fraction of mesozooplankton carbon released to labile particulate pool ($0 \leq$ FLPOCLZ ≤ 1)
3	FRPOCLZ	Real	Fraction of mesozooplankton carbon released to refractory particulate pool ($0 \leq$ FRPOCLZ ≤ 1)
1	FNH4LZ	Real	Fraction of mesozooplankton nitrogen released as ammonium ($0 \leq$ FNH4LZ ≤ 1)
2	FDONLZ	Real	Fraction of mesozooplankton nitrogen released to dissolved organic pool ($0 \leq$ FDONLZ ≤ 1)
3	FLPONLZ	Real	Fraction of mesozooplankton nitrogen released to labile particulate pool ($0 \leq$ FLPONLZ ≤ 1)
4	FRPONLZ	Real	Fraction of mesozooplankton nitrogen released to refractory particulate pool ($0 \leq$ FRPONLZ ≤ 1)
1	FPO4LZ	Real	Fraction of mesozooplankton phosphorus released as phosphate ($0 \leq$ FPO4LZ ≤ 1)
2	FDOPLZ	Real	Fraction of mesozooplankton phosphorus released to dissolved organic pool ($0 \leq$ FDOPLZ ≤ 1)
3	FLPOPLZ	Real	Fraction of mesozooplankton phosphorus released to labile particulate pool ($0 \leq$ FDOPLZ ≤ 1)

4	FRPOPLZ	Real	Fraction of mesozooplankton phosphorus released to refractory particulate pool ($0 \leq$ FDOPLZ ≤ 1)
1	FRSALZ	Real	Fraction of silica released by mesozooplankton to dissolved pool ($0 \leq$ FRSALZ ≤ 1)

Example

```
  CTSZ   KHCSZ DOCRTSZ MZEROSZ
  0.01    0.05     2.0     4.0

 ANCSZ   APCSZ  AOCRSZ
  0.20   0.020    2.67

 UBCSZ   UBDSZ   UBGSZ    UDSZ    ULSZ    URSZ
   0.0     1.0     1.0     0.1     0.1     0.1

  TMSZ  KTGSZ1  KTGSZ2    TRSZ   KTBSZ   TPRSZ  KTPRSZ
  25.0  0.0035   0.025    20.0  0.0693    20.0  0.0693

FDOCSZ FLPOCSZ FRPOCSZ
  0.25    0.50    0.25

FHN4SZ  FDONSZ FLPONSZ FRPONSZ
  0.55    0.20   0.200   0.050

FPO4SZ  FDOPSZ FLPOPSZ FRPOPSZ
  0.50    0.40   0.070   0.030

FRSASZ
  0.55

  CTLZ   KHCLZ DOCRTLZ MZEROLZ
  0.05   0.175     2.0     4.0

 ANCLZ   APCLZ  AOCRLZ
  0.20   0.020    2.67

 UBCLZ   UBDLZ   UBGLZ   USZLZ    ULLZ    URLZ
   0.0     1.0     1.0     1.0     0.1     0.1

  TMLZ  KTGLZ1  KTGLZ2    TRLZ   KTBLZ   TPRLZ  KTPRLZ
  25.0   0.008   0.030    20.0  0.0693    20.0  0.0693

FDOCLZ FLPOCLZ FRPOCLZ
  0.25    0.50    0.25

FHN4LZ  FDONLZ FLPONLZ FRPONLZ
  0.55    0.20   0.200   0.050

FPO4LZ  FDOPLZ FLPOPLZ FRPOPLZ
  0.50    0.40   0.070   0.030

FRSALZ
  0.55
```

Spatially-Varying Parameters

Zooplankton grazing, respiration, and predation losses may be applied uniformly throughout the domain or may be varied spatially. The option to vary these spatially is useful for large systems in which different communities are

present e.g. freshwater vs. saltwater. Each group of the spatially-varying parameters follows the same convention – a blank line, a parameter list, and a line of parameter values. The first parameter list (//8X,8A8) specifies spatially-uniform or varying parameter assignment and determines if input values should be echoed to the output file. For spatially-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to spatially-varying parameter assignment. To print entries to the output file, enter the character string ' ALL'. The second parameter list specifies parameter values (//(8X,5F8.2)). One line of parameter values is required for CONSTANT specification. Otherwise, one line must be entered for each cell in the model grid. For convenience, the cell number may be entered in the first eight columns. This number is not read into the program. Parameters are understood to be in order starting from cell 1 up to the highest cell number.

Field	Name	Value	Description
1	SPVAR1	Character	Spatially uniform (CONSTANT) or varying parameter specification for microzooplankton
2	PRINT1	Character	Print (ALL) or do not print out microzooplankton parameters
1	RMAXSZ	Real	Maximum ration for microzooplankton (g prey C g^{-1} zooplankton C d^{-1})
2	ESZ	Real	Microzooplankton assimilation efficiency ($0 \leq ESZ \leq 1$)
3	RFSZ	Real	Microzooplankton fraction of assimilated prey lost to respiration ($0 \leq RFSZ \leq 1$)
4	BMRSZ	Real	Microzooplankton basal metabolism at reference temperature (d^{-1})
5	PRSZ	Real	Non-specific predation on microzooplankton (m^3 g^{-1} C d^{-1})
1	SPVAR2	Character	Spatially uniform (CONSTANT) or varying parameter specification for mesozooplankton
2	PRINT2	Character	Print (ALL) or do not print out mesozooplankton parameters
1	RMAXLZ	Real	Maximum ration for mesozooplankton (g prey C g^{-1} zooplankton C d^{-1})
2	ELZ	Real	Mesozooplankton assimilation efficiency ($0 \leq ELZ \leq 1$)
3	RFLZ	Real	Mesozooplankton fraction of assimilated prey lost to respiration ($0 \leq RFLZ \leq 1$)
4	BMRLZ	Real	Mesozooplankton basal metabolism at reference temperature (d^{-1})
5	PRLZ	Real	Predation on mesozooplankton by higher trophic levels (m^3 g^{-1} C d^{-1})

Example

```
ZOOPL 1   SPVAR1  PRINT1
        CONSTANT      NO

     BOX  RMAXSZ     ESZ    RFSZ   BMRSZ    PRSZ
       1   2.250   0.300   0.500   0.254   0.000

ZOOPL 2   SPVAR2  PRINT2
        CONSTANT      NO

     BOX  RMAXLZ     ELZ    RFLZ   BMRLZ    PRLZ
       1   1.750   0.300   0.070   0.186   2.000
```

Temporally-Varying Parameters

Zooplankton predation losses may be multiplied by a constant to create a piecewise predation function. This option is appropriate if zooplankton predators (e.g. migratory fish) are present at specific seasons. Each group of the temporally-varying parameters follows the same convention – a blank line, a parameter list, and a line of parameter values. The first parameter list (//8X,8A8) specifies temporally-uniform or varying parameter assignment and determines if input values should be echoed to the output file. For temporally-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to temporally-varying parameter assignment. To print entries to the output file, enter the character string ' ALL'. The second parameter list specifies parameter values (//(16X,F8.0)). One line of parameter values is required for CONSTANT specification. In this case, the value 1.0 should be entered for TVPRSZ or TVPRLZ. Otherwise, 366 lines must be entered – one for each day of the year. For convenience, the day may be entered in the first 16 columns. This number is not read into the program. Parameters are understood to be in order starting from day 1.

Field	Name	Value	Description
1	TVARSZ	Character	Temporally uniform (CONSTANT) or varying parameter specification for microzooplankton
2	PRINTSZ	Character	Print (ALL) or do not print out microzooplankton parameters
1	TVPRSZ	Real	Mutiplier for predation on microzooplankton by predators other than mesozooplankton ($0 \leq TVPRSZ \leq 1$)
1	TVARLZ	Character	Temporally uniform (CONSTANT) or varying parameter specification for mesozooplankton
2	PRINTLZ	Character	Print (ALL) or do not print out mesozooplankton parameters
1	TVPRLZ	Real	Mutiplier for predation on mesozooplankton by higher trophic levels ($0 \leq TVPRLZ \leq 1$)

Example

```
TVARSZ PRINTSZ
  CONSTANT     ALL

       DAY  TVPRSZ
 1           1.000

   TVARLZ PRINTLZ
  CONSTANT     ALL

       DAY  TVPRLZ
 1           1.000
```

Temperature Effect on Mesozooplankton Grazing

The zooplankton model was developed for Chesapeake Bay. Several mesozooplankton species predominate in the bay, depending on location and season. In particular, the spring community in the mainstem bay, largely *Eurytemora affinis* and *Acartia hudsonica*, differs from the summer community, predominantly *Acartia tonsa*. We attempted to mimic the varying predation pressure exerted by these two groups through specification of a piecewise temperature function on grazing. This function overwrites the exponential dependence specified with parameters TMLZ, KTGLZ1, KTGLZ2. Thirty-five multipliers are specified, corresponding to degrees from 0 to 34 C. These multipliers operate on parameter RMAXLZ. The user can specify an exponential relationship by specifying 35 multipliers calculated to represent an exponential function. Alternately, functions with one or two temperature maxima can be employed. Or, the adventurous user can go into the model code and restore the original dependence on TMLZ, KTGLZ1, KTGLZ2.

A title line indicates that the temperature function follows. The format statement that reads the temperature multipliers, f(T), is (//(8X,8F8.0)). For convenience, the temperature may be placed in the first eight columns. This field is not read into the model, however. The code requires 35 values, spaced one degree apart and starting with zero degrees C.

Example

```
      f(T)
 0   0.060
 1   0.075
 2   0.093
 3   0.113
 4   0.137
 5   0.165
 6   0.197
 7   0.233
 8   0.272
 9   0.316
10   0.363
11   0.414
12   0.467
13   0.523
14   0.580
15   0.638
16   0.695
17   0.750
18   0.802
19   0.850
```

```
20   0.894
21   0.931
22   0.960
23   0.982
24   0.996
25   1.000
26   0.970
27   0.887
28   0.763
29   0.619
30   0.472
31   0.340
32   0.230
33   0.147
34   0.088
35   0.050
```

Pathogens and Toxicants

Introduction

At the request of the sponsor, a pathogen and two toxicants were added to the model code. The pathogen is activated in the present application and represents fecal coliform bacteria. The two toxicants are coded in a generalized format and are not presently activated. The general formulation is intended to provide a rapid screening tool. The formulation also provides the foundation for a more detailed application, should this be desired.

Conservation of Mass Equation

The foundation of CE-QUAL-ICM is the solution to the three-dimensional mass-conservation equation for a control volume. Control volumes correspond to cells on the model grid. CE-QUAL-ICM solves, for each volume and for each state variable, the equation:

$$\frac{\delta V_j \bullet C_j}{\delta t} = \sum_{k=1}^{n} Q_k \bullet C_k + \sum_{k=1}^{n} A_k \bullet D_k \bullet \frac{\delta C}{\delta x_k} + \Sigma S_j$$

Equation 1

in which:

V_j = volume of j^{th} control volume (m^3)
C_j = concentration in j^{th} control volume (g m^{-3})
t, x = temporal and spatial coordinates
n = number of flow faces attached to j^{th} control volume
Q_k = volumetric flow across flow face k of j^{th} control volume (m^3 s^{-1})
C_k = concentration in flow across face k (g m^{-3})
A_k = area of flow face k (m^2)
D_k = diffusion coefficient at flow face k (m^2 s^{-1})
S_j = external loads and kinetic sources and sinks in j^{th} control volume (g s^{-1})

Solution of Equation 1 on a digital computer requires discretization of the continuous derivatives and specification of parameter values. The equation is solved using the QUICKEST algorithm (Leonard 1979) in the horizontal plane and a Crank-Nicolson scheme in the vertical direction. Discrete time steps, determined by computational stability requirements, are .15 minutes.

The remainder of this chapter is devoted to detailing the kinetics sources and sinks and to reporting parameter values. For notational simplicity, the transport terms are dropped in the reporting of kinetics formulations.

Pathogen

The pathogen undergoes temperature-dependent first-order decay:

$$\frac{\delta}{\delta t} PATH = - Kpath \bullet f(T) \bullet PATH$$

Equation 2

in which:

PATH = pathogen concentration (mpn 100 mL^{-1})
Kpath = decay rate at reference temperature T (d^{-1})

For Lake Washington, the pathogen decay rate is 0.1 d^{-1} at 20 ^{o}C. The temperature function, f(T), is an exponential relationship in which decay rate doubles for a 10^{o} increase in temperature (Figure 1).

Toxicants

The two toxicants are subject to identical kinetics processes (Figure 2) including:

Decay
Volatilization
Partitioning to solids
Settling
Burial

Toxicant 1 partitions to inorganic solids (which can be configured to represent a metal). Toxicant 2 partitions to particulate organic carbon. Toxicant not lost through decay or volatilization may settle to the bottom sediments. Within the sediments, toxicant is subject to decay and burial. Dissolved toxicant diffuses in either direction across the sediment-water interface.

Reactions in the Water Column

The basic representations for the two toxicants are identical:

$$\frac{\delta}{\delta t} TOX = -Ktox \bullet f(T) \bullet TOX - Kvol \bullet Fd \bullet \frac{TOX}{\Delta z}$$
$$- Ws \bullet \frac{\delta}{\delta z} (Fp \bullet TOX)$$

Equation 3

in which:

TOX = toxicant concentration (g m^{-3})
Ktox = decay rate at reference temperature T (d^{-1})
Kvol = volatilization rate (m d^{-1})
Fd = dissolved fraction of total toxicant ($0 \leq Fd \leq 1$)
Fp = particulate fraction of total toxicant (= 1 – Fd)
Ws = particle settling velocity (m d^{-1})
Δz = surface layer thickness (m)

The decay rate increases as an exponential function of temperature. The volatilization formulation assumes that toxicant concentration in the atmosphere is negligible.

Particulate and Dissolved Fractions

For Toxicant 1, the particulate fraction is:

$$Fp = \frac{KADtox1 \bullet ISS}{1 + KADtox1 \bullet ISS}$$

Equation 4

in which:

KADtox1 = toxicant 1 partition coefficient (m^3 g^{-1})
ISS = inorganic solids concentration (g m^{-3})

For Toxicant 2, the particulate fraction is:

$$Fp = \frac{KADtox2 \bullet (B + LPOC + RPOC)}{1 + KADtox2 \bullet (B + LPOC + RPOC)}$$

Equation 5

in which:

KADtox2 = toxicant 2 partition coefficient (m^3 g^{-1} C)

B = algal biomass (g C m^{-3})
LPOC = labile particulate organic carbon (g C m^{-3})
RPOC = refractory particulate organic carbon (g C m^{-3})

The dissolved fraction, for both toxiciants, is:

$$Fd = 1 - Fp$$

Equation 6

Settling

The appropriate settling velocity for Toxicant 1 is the inorganic solids settling velocity, Wiss. The settling velocities for the multiple components to which Toxicant 2 partitions may vary. The settling term is weighted by the product of the component settling velocities and concentrations:

$$Ws \bullet \frac{\delta}{\delta z}(Fp \bullet TOX) =$$
$$\frac{\delta}{\delta z} KADtox2 \bullet \frac{WSa \bullet B + WSl \bullet LPOC + WSr \bullet RPOC}{1 + KADtox2 \bullet (B + LPOC + RPOC)} \bullet TOX$$

Equation 7

in which:

WSa = algal settling velocity (m d^{-1})
WSl = labile particulate organic carbon settling velocity (m d^{-1})
WSr = refractory particulate organic carbon settling velocity (m d^{-1})

Reactions in the Sediments

Bed sediments are envisioned as a single, well-mixed layer (Figure 2). Toxicants are exchanged with the overlying water through settling of the particulate fraction and diffusion of the dissolved fraction. Within the sediments, toxicants undergo decay and burial to deep, inactive sediments. The mass-balance equations for both toxicants are identical:

$$H \bullet \frac{\delta}{\delta t} TOXsed = -(Ktoxsed \bullet f(T) \bullet H + Wbur) \bullet TOXsed$$
$$+ Wnet \bullet Fpw \bullet TOXw - s \bullet (Fdsed \bullet TOXsed - Fdw \bullet TOXw)$$

Equation 8

in which:

TOXsed = bulk concentration of toxicant in sediments (g m^{-3})
TOXw = concentration of toxicant in overlying water (g m^{-3})
H = thickness of active sediment layer (m)
Ktoxsed = decay rate in sediments (d-1)
Wbur = burial rate to deep, inactive sediments (m d^{-1})
Wnet = net settling velocity of solids into sediments (m d^{-1})
s = sediment-water mass transfer velocity (m d^{-1})
Fdw = dissolved fraction in the overlying water ($0 \leq Fdw \leq 1$)
Fpw = particulate fraction in water (= 1 - Fdw)
Fdsed = dissolved fraction in sediments ($0 \leq Fdsed \leq 1$)

Decay rates and partition coefficients within the sediments may vary from those specified for the water column. For Toxicant 1, the dissolved fraction within the sediments is:

$$Fdsed = \frac{1}{1 + KADsedtox1 \bullet ISSsed}$$

Equation 9

in which:

KADsedtox1 = toxicant 1 partition coefficient in sediments (m^3 g^{-1})
ISSsed = bulk inorganic solids concentration in sediments (g m^{-3})

For Toxicant 2, the dissolved fraction is:

$$Fdsed = \frac{1}{1 + KADsedtox2 \bullet (G1 + G2 + G3)}$$

Equation 10

In which

KADsedtox2 = toxicant 2 partition coefficient in sediments (m^3 g^{-1} C)
G1 = labile organic carbon concentration in sediments (g C m^{-3})
G2 = refractory organic carbon concentration in sediments (g C m^{-3})
G3 = inert organic carbon concentration in sediments (g C m^{-3})

The bulk sediment solids concentration is an input to the diagenesis model. The sediment carbon concentrations are computed within the sediment model. The sediment-water mass-transfer velocity can be specified as an input to the toxicant model or the value computed in the diagenesis model can be employed.

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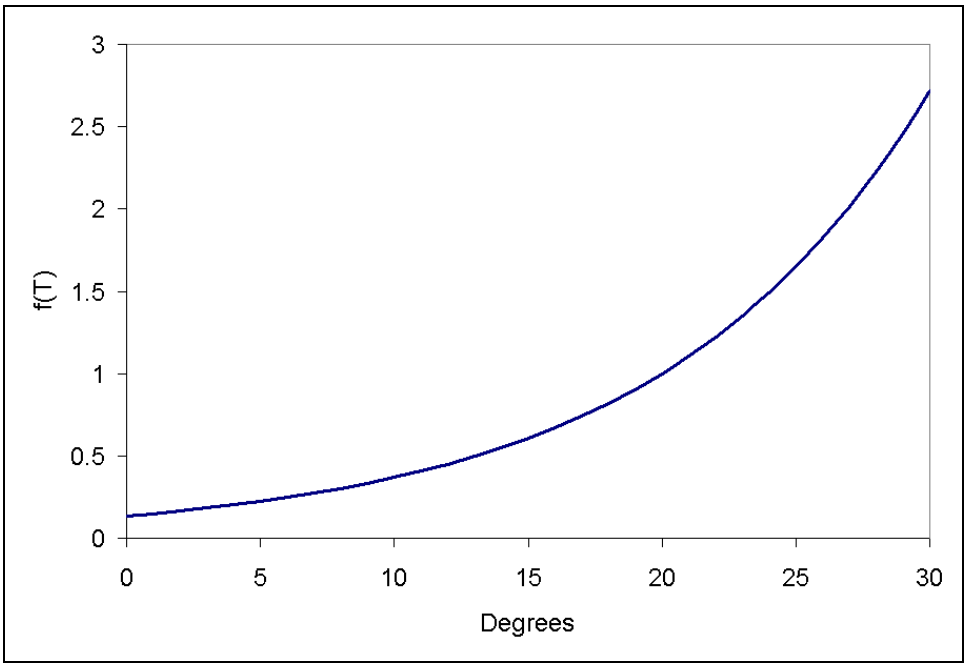

Figure 1. Effect of temperature on pathogen decay

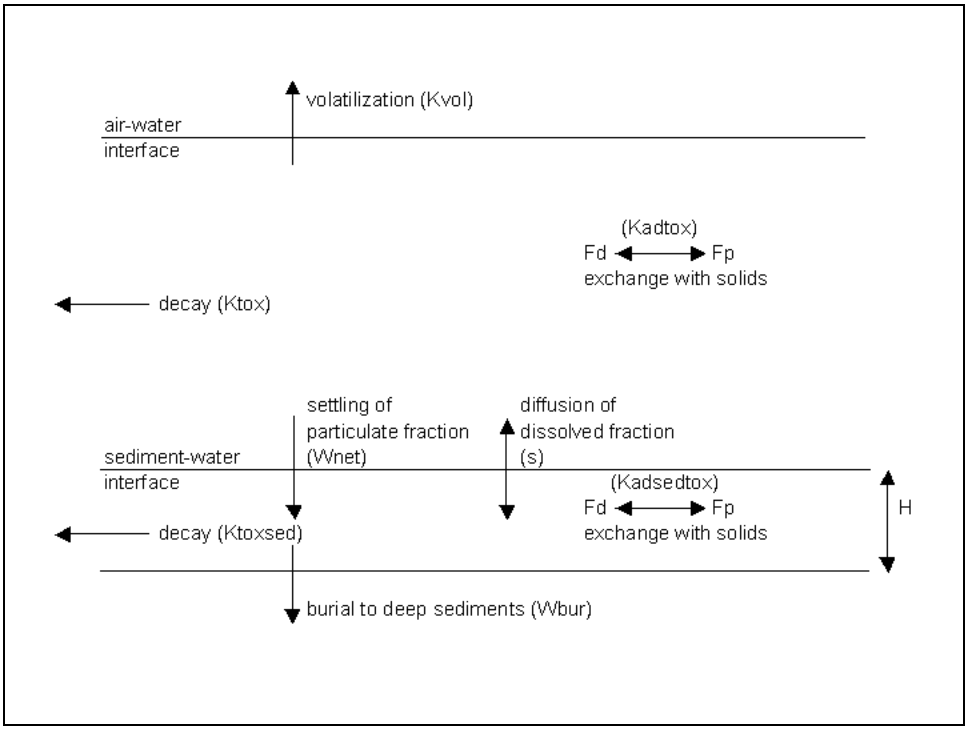

Figure 2. Schematic of toxicant model

Sediment-Water Interactions

Introduction

Exchange of material between the water column and benthic sediments is an important component of the eutrophication process. Sediment oxygen demand may comprise a substantial fraction of total system oxygen consumption. Over lengthy time scales (e.g. years to decades), the sediments are an ultimate sink of nutrients and other substances discharged to the water column. Over lesser time scales (e.g. seasons to years), however, sediment release of previously-deposited nutrients can be a net source to the water column.

Within the model, transfer of particulate matter from water to sediments is treated through specification of a settling velocity. Two options are available for determination of sediment oxygen consumption and sediment nutrient releases. The first option employs user-specified fluxes. Basic relationships are provided that express the influence of conditions in the water column on the specified fluxes. The second option is employment of a fully-predictive sediment submodel that computes fluxes based on deposition of organic particles and other factors.

Excellent calibration of the water-quality model can be achieved with employment of user-specified fluxes. This option provides limited insight into sediment response to alterations in loading and other factors, however. Employment of the sediment submodel provides rational predictions of sediment response to environmental alterations. Employment of the submodel vastly increases information requirements and computation time compared to employment of user-specified fluxes.

User-Specified Fluxes

The model employs the convention that positive fluxes are from sediment to water and negative fluxes are from water to sediment. Fluxes of dissolved organic matter, ammonium, phosphate, and chemical oxygen demand are most often from sediments to water and are positive quantities. Nitrate commonly passes in both directions across the sediment-water interface and may be positive or negative. Since oxygen moves from water to sediments, sediment oxygen consumption is represented as a negative quantity.

Dissolved Organic Carbon, Ammonium, Phosphate

The model accounts for effects of temperature (Figure 1) on user-specified sediment-water fluxes of dissolved organic carbon, ammonium, and phosphate. The relationship is:

$$BENx = BENxb \cdot e^{KSx \cdot (T - TRSx)}$$

Equation 1

in which:

BENx = benthic flux of substance x at temperature T (gm m^{-2} day^{-1})
BENxb = benthic flux of substance x specified at temperature TRSx (gm m^{-2} day^{-1})
KSx = effect of temperature on flux of substance x ($C^{o\,-1}$)
T = temperature (C^o)
TRSx = reference temperature for specification of benthic flux (C^o)

Nitrate

Movement of nitrate between water and sediments is strongly influenced by concentration of nitrate in the water column. When nitrate is abundant in the water column, nitrate usually diffuses from overlying water into the sediments where it is denitrified to gaseous form. When nitrate is absent from the water column, small quantities of nitrate may diffuse from sediment interstitial water into the overlying water. The model allows for user-specified nitrate flux and provides a function (Figure 2) that relates flux to concentration:

$$BENNO_3 = BENNO_3b + MTC \cdot (SEDNO_3 - NO_3) \cdot e^{KSNO_3 \cdot (T - TRSNO_3)}$$

Equation 2

in which:

$BENNO_3$ = sediment-water nitrate flux (gm N m^{-2} day^{-1})
$BENNO_3b$= specified sediment-water nitrate flux (gm N m^{-2} day^{-1})
MTC = sediment-water mass transfer coefficient (m day^{-1})
$SEDNO_3$ = nitrate concentration in interstitial water (gm m^{-3})
NO_3 = nitrate concentration in water overlying sediments (gm m^{-3})
$KSNO_3$ = effect of temperature on denitrification rate ($C^{o\,-1}$)
$TRSNO_3$ = reference temperature for specification of denitrification rate (C^o)

In typical model employment, the user specifies the nitrate flux, if known, or relies on the model to compute flux as a function of nitrate in the water column.

Sediment Oxygen Consumption

Oxygen consumption in the sediments depends upon water-column temperature and oxygen availability. As temperature increases, respiration in the sediment increases. Sediment oxygen consumption is reduced as oxygen concentration in the overlying water decreases. The model accounts for these influences through the relationship:

$$BENDO = \frac{DO}{KHso + DO} \cdot BENDOb \cdot e^{KSo \cdot (T - TRSo)}$$

Equation 3

in which:

BENDO = sediment oxygen consumption (gm m^{-2} day^{-1})
$BENDO_b$ = sediment oxygen consumption under conditions of unlimited oxygen availability, specified at temperature TRSo (gm m^{-2} day^{-1})
KHso = dissolved oxygen concentration at which sediment oxygen consumption is halved (gm m^{-3})
KSo = effect of temperature on sediment oxygen consumption ($C^{o\ -1}$)
TRSo = reference temperature for specification of sediment oxygen consumption (C^{o})

Chemical Oxygen Demand

The processes that create sediment oxygen demand are little affected by the concentration of oxygen in the overlying water. When oxygen is unavailable to fulfill sediment oxygen demand, the demand is exported to the water column. The exported demand may be in the form of reduced iron, manganese, or sulfide, which are represented in the model as chemical oxygen demand. The model allows for user-specified sediment release of chemical oxygen demand and provides a function which computes additional release as oxygen consumption in the sediments is constrained:

$$BENCOD = BENCODb - \frac{KHso}{KHSO + DO} \cdot BENDOb \cdot e^{KSo \cdot (T - TRSo)}$$

Equation 4

in which:

BENCOD = sediment flux of chemical oxygen demand (gm m^{-2} day^{-1})
BENCODb = specified sediment-water flux of chemical oxygen demand (gm m^{-2} day^{-1})

In typical model employment, the user specifies the flux of chemical oxygen demand, if known, or relies on the model to compute flux as a function of

sediment oxygen consumption and dissolved oxygen in the water column. The computed flux is negligible when DO >> KHso (Figure 3). When dissolved oxygen is absent from the water column, oxygen demand equivalent to maximum specified sediment consumption is released to the water as chemical oxygen demand.

Dissolved Organic Nitrogen and Phosphorus

The model allows for user-specified fluxes of dissolved organic nitrogen and dissolved organic phosphorus. Sediment release of these substances is small and erratic. The model provides no functions that modify the user-specified basic fluxes.

Parameter Evaluation

Base fluxes and influences of temperature and other factors are best determined from observations collected in the prototype system. Table 1 lists observations from several systems that may be employed as starting values when no observations are available. Suggested starting values for parameters in the functions that relate sediment-water fluxes to conditions in the water column are listed in Table 2.

Predictive Sediment Submodel

The predictive benthic sediment model applied to Lake Washington was first developed for use in Chesapeake Bay (DiToro and Fitzpatrick 1993). Management of the bay required a model with two fundamental capabilities:

- Predict effects of management actions on sediment-water exchange processes, and

- Predict time scale for alterations in sediment-water exchange processes.

The model (Figure 4, Table 3) is driven by net settling of organic matter from the water column to the sediments. In the sediments, the model simulates the diagenesis (decay) of the organic matter. Diagenesis produces oxygen demand and inorganic nutrients. Oxygen demand, as sulfide (in saltwater) or methane (in freshwater), takes three paths out of the sediments: export to the water column as chemical oxygen demand, oxidation at the sediment-water interface as sediment oxygen demand, or burial to deep, inactive sediments. Inorganic nutrients produced by diagenesis take two paths out of the sediments: release to the water column, or burial to deep, inactive sediments.

The formulation of the diagenesis model is too extensive to repeat here. Initial model documentation was provided by DiToro and Fitzpatrick (1993). More accessible, recent, documentation may be found in DiToro (2001). Details of the sediment model, required to understand the coupling of the sediment submodel to the model of the water column, are provided in this chapter.

Table 1
Observed Sediment-Water Fluxes

Ammonium, mg m^{-2} day^{-1}	Nitrate, mg m^{-2} day^{-1}	Phosphate, mg m^{-2} day^{-1}	Silica, mg m^{-2} day^{-1}	SOD, gm m^{-2} day^{-1}	System
10 to 280	-40 to 100	-3 to 30		-1.5 to -3.5	Chesapeake Bay (Boynton and Kemp 1985)
			67 to 670		Chesapeake Bay (D'Elia et al. 1983)
-1 to 90	-20 to 15	-7 to 31		-0.1 to -2.6	Narragansett Bay (Hale 1975)
0 to 150	0 to 2	-6 to 34		-0.6 to -2.4	Neuse and South Rivers, NC (Fisher et al. 1982)
-40 to 360	-100 to 80	-19 to 124		-0.1 to -2.7	Potomac Estuary (Callender and Hammond 1982)
-35 to 530	-230 to 30	1 to 220		-0.5 to -4.1	Patuxent Estuary (Boynton et al 1980)

Table 2
Parameters in Sediment-Water Flux Relationships

Parameter	Suggested Range
KSx	0.04 to 0.07 $C^{o\ -1}$
MTC	0.05 to 0.15 m day^{-1}
$SEDNO_3$	0 to 0.05 gm m^{-3}
KHso	1 to 2 gm m^{-3}

Coupling With the Sediment Diagenesis Model

Benthic sediments are represented as two layers with a total depth of 10 cm (Figure 5). The upper layer, in contact with the water column, may be oxic or anoxic depending on dissolved oxygen concentration in the water. The lower layer is permanently anoxic. The thickness of the upper layer is determined by the penetration of oxygen into the sediments. At its maximum thickness, the oxic layer depth is only a small fraction of the total.

Table 3
Sediment Model State Variables and Fluxes

State Variable	Sediment-Water Flux
Temperature	
Particulate Organic Carbon	Sediment Oxygen Demand
Sulfide/Methane	Release of Chemical Oxygen Demand
Particulate Organic Nitrogen	
Ammonium	Ammonium Flux
Nitrate	Nitrate Flux
Particulate Organic Phosphorus	
Phosphate	Phosphate Flux
Particulate Biogenic Silica*	
Available Silica*	Silica Flux*

* Not activated in Lake Washington

The sediment model consists of three basic processes. The first is deposition of particulate organic matter from the water column to the sediments. Due to the negligible thickness of the upper layer, deposition proceeds from the water column directly to the lower, anoxic layer. Within the lower layer, organic matter is subject to the second basic process, diagenesis (or decay). The third basic process is flux of substances produced by diagenesis to the upper sediment layer, to the water column, and to deep, inactive sediments. The flux portion of the model is the most complex. Computation of flux requires consideration of reactions in both sediment layers, of partitioning between particulate and dissolved fractions in both layers, of sedimentation from the upper to lower layer and from the lower layer to deep inactive sediments, of particle mixing between layers, of diffusion between layers, and of mass transfer between the upper layer and the water column.

The water quality and sediment models interact on a time scale equal to the integration time step of the water quality model. After each integration, predicted particle deposition, temperature, nutrient and dissolved oxygen concentrations are passed from the water quality model to the sediment model. The sediment model computes sediment-water fluxes of dissolved nutrients and oxygen based on predicted diagenesis and concentrations in the sediments and water. The computed sediment-water fluxes are incorporated by the water quality model into appropriate mass balances and kinetic reactions.

Deposition

Deposition is one process that couples the model of the water column with the model of the sediments. Consequently, deposition is represented in both the sediment and water-column models. In the water column, deposition is represented with a modification of the mass-balance equation applied only to cells that interface the sediments:

$$\frac{\delta C}{\delta t} = [transport] + [kinetics] + \frac{WS}{\Delta z} \bullet C_{up} - \frac{W_{net}}{\Delta z} \bullet C$$

Equation 5

in which:

C concentration of particulate constituent in cell above sediments (g m^{-3})
WS = settling velocity in water column (m d^{-1})
Cup = constituent concentration two cells above sediments (g m^{-3})
Wnet = net settling to sediments (m d^{-1})
Δz = cell thickness (m)

Net settling to the sediments may be less than or equal to settling in the water column. Sediment resuspension is implied when settling to the sediments is less than settling through the water column.

Diagenesis

Organic matter in the sediments is divided into three G classes or fractions, in accordance with principles established by Westrich and Berner (1984). Division into G classes accounts for differential decay rates of organic matter fractions. The G1, labile, fraction has a half-life of 20 days. The G2, refractory, fraction has a half-life of one year. The G3, inert, fraction undergoes no significant decay before burial into deep, inactive sediments. Each G class has its own mass-conservation equation:

$$H \bullet \frac{\delta Gi}{\delta t} = W_{net} \bullet f_i \bullet C - W \bullet Gi - H \bullet K_i \bullet Gi \bullet \theta_i^{(T-20)}$$

Equation 6

in which:

H = total thickness of sediment layer (m)
Gi = concentration organic matter in G class i (g m^{-3})
f_i = fraction of deposited organic matter assigned to G class i
W = burial rate (m d^{-1})
K_i = decay rate of G class i (d^{-1})
θ_i = constant that expresses effect of temperature on decay of G class i

Since the G3 class is inert, $K_3 = 0$.

Sediment-Water Flux

The exchange of dissolved substances between the sediments and water column is driven by the concentration difference between the surface sediment layer and the overlying water. Flux may be in either direction across the sediment-water interface, depending on concentration gradient. Sediment-water flux is computed within the diagenesis model as the product of concentration difference and an internally-computed mass-transfer coefficient. In the water column, sediment-water exchange of dissolved substances is represented with a modification of the mass-balance equation applied only to cells that interface with bottom sediments:

$$\frac{\delta C}{\delta t} = [transport] + [kinetics] + \frac{BENFLX}{\Delta z}$$

Equation 7

in which:

BENFLX = sediment-water flux of dissolved substance (g m^{-2} d^{-1})

By convention, positive fluxes are from sediment to water. Negative fluxes, including sediment oxygen demand, are from water to sediments.

Parameter Specification

Coupling with the sediment model requires specification of net settling rates, of the G splits of organic matter, and of burial rates.

Net Settling Rates

Net settling for inorganic solids and detritus was specified as half the settling rate in the water column. The lower net settling rates, 0.5 m d^{-1} for solids and 0.4 m d^{-1} for detritus, were specified in an attempt to reproduce high particle concentrations observed near the bottom of the water column. Net settling for algae was the same as settling through the water column, 0.1 m d^{-1}.

Assignment to G Classes

Upon deposition in the sediments, state variables representing particulate organic matter in the water quality model required conversion into sediment model state variables. The water quality model considered two classes of particulate organic matter: labile and refractory. The sediment model was based on three classes of organic particles: labile (G1), refractory (G2), and inert (G3). Labile particles from the water quality model were transferred directly into the G1 class in the sediment model. Refractory particles from the water quality model had to be split into G2 and G3 fractions upon entering the sediments. Algae settling directly to the sediments also required routing into sediment model state variables. Guidance for the splits (Table 4) was obtained from phytoplankton decomposition experiments (Westrich and Berner 1984). Planktonic particulate organic carbon was found to be 50% labile, 16% refractory, and 34% non-reactive.

Table 4
Routing Organic Particles into Sediment Classes

WQM Variable	Carbon			Nitrogen			Phosphorus		
	% G1	% G2	% G3	% G1	% G2	% G3	% G1	% G2	% G3
Labile Particles	100			100			100		
Refractory Particles		32	68		32	68		32	68
Algae	50	16	34	50	16	34	50	16	34

Burial Rates

The burial rate in the sediment model, as applied to central Chesapeake Bay, is 0.25 cm yr^{-1}. Kuivila and Murray (1984) cite sedimentation rates of 0.31 to 0.53 cm yr^{-1} in Lake Washington. In view of the similarity in burial rates and the minor role of this rate in the model, the burial rate of 0.25 cm yr^{-1} was retained for this application.

Sediment Model Parameters

With few exceptions, the typical user will not want to alter the parameters evaluated in the initial Chesapeake Bay application of the diagenesis model. For one reason, most parameters have been found to be transferable

between systems. For another, parameter evaluation requires a large observational data base that is difficult and expensive to assemble. The user will more likely alter the parameters that determine the coupling between the models of the water column and sediments. We have, however, found a few areas in which diagenesis parameters require alteration to represent specific systems. In the initial model application, nitrification and denitrification rates were increased (≈50% to 100%) in the freshwater portions of Chesapeake Bay relative to the saline portions (Cerco and Cole 1994). In applying the diagenesis model to multiple systems, DiToro (2001) noted the phosphorus partition coefficients frequently required revision. We have had the same experience with our own applications. The Chesapeake Bay partition coefficients were halved for the Lake Washington application. Phosphorus partition coefficients were reduced from 30,000 L kg^{-1} to 7,500 L kg^{-1} in the surface sediments and from 100 L kg^{-1} to 50 L kg^{-1} in the subsurface sediments. The partition coefficients employed in Lake Washington are low compared to the range reported by DiToro. The low partition coefficients imply Lake Washington sediments have low phosphorus retention relative to the other systems. The reduction of partition coefficients is the opposite of our experience to date. We usually increase the partition coefficients for freshwater systems, relative to the original estuarine application. We cannot speculate on the apparent difference in properties for Lake Washington.

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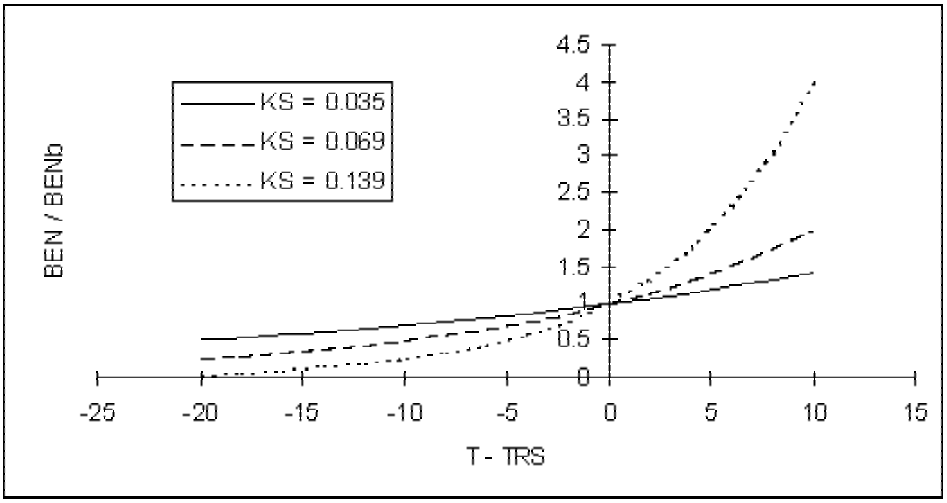

Figure 1. Effect of temperature on specified fluxes

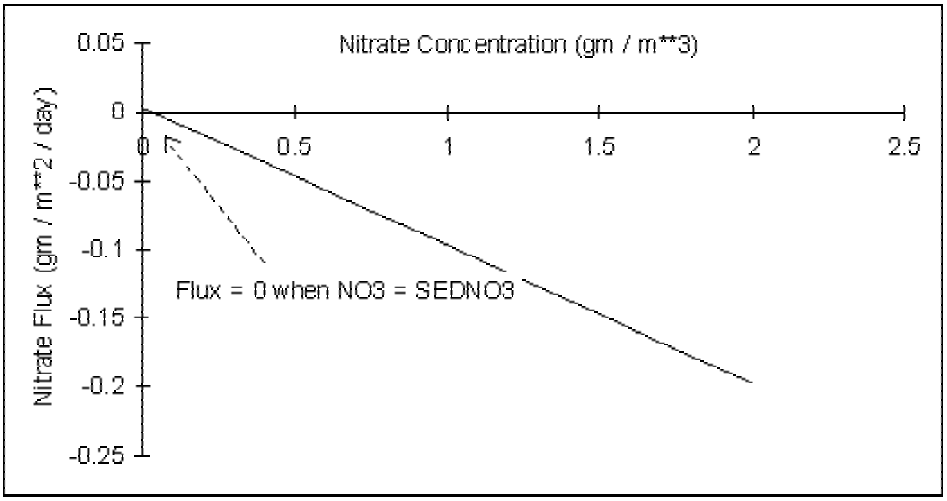

Figure 2. Effect of nitrate concentration on sediment-water nitrate flux

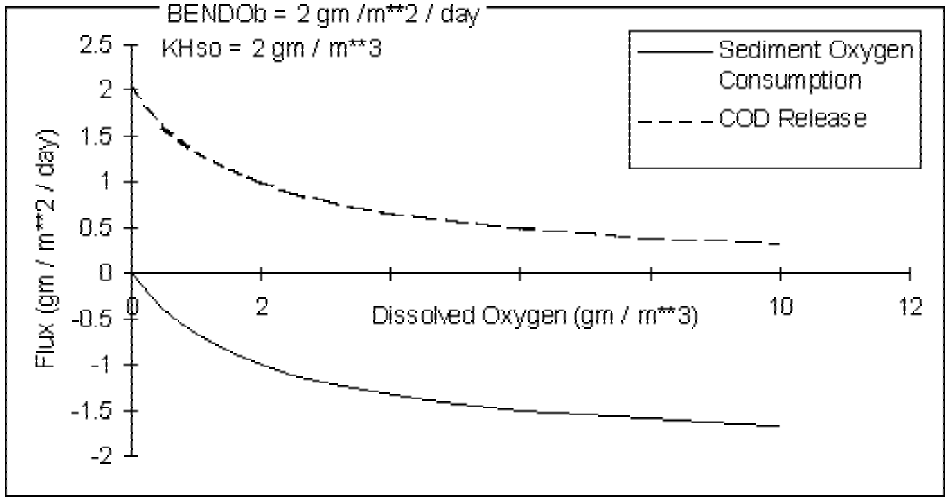

Figure 3. Effect of dissolved oxygen on sediment oxygen consumption and COD release

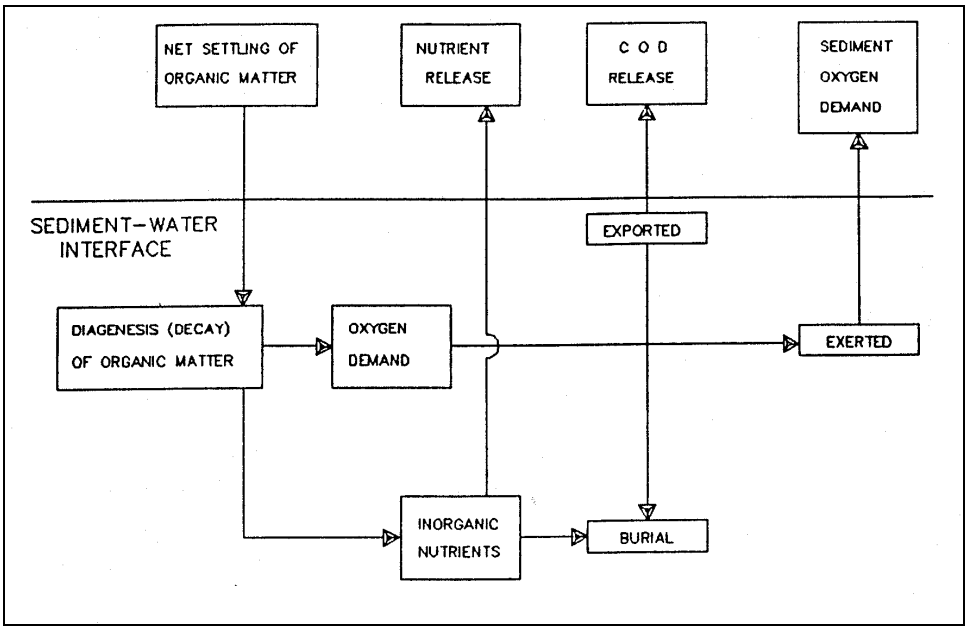

Figure 4. Sediment model schematic

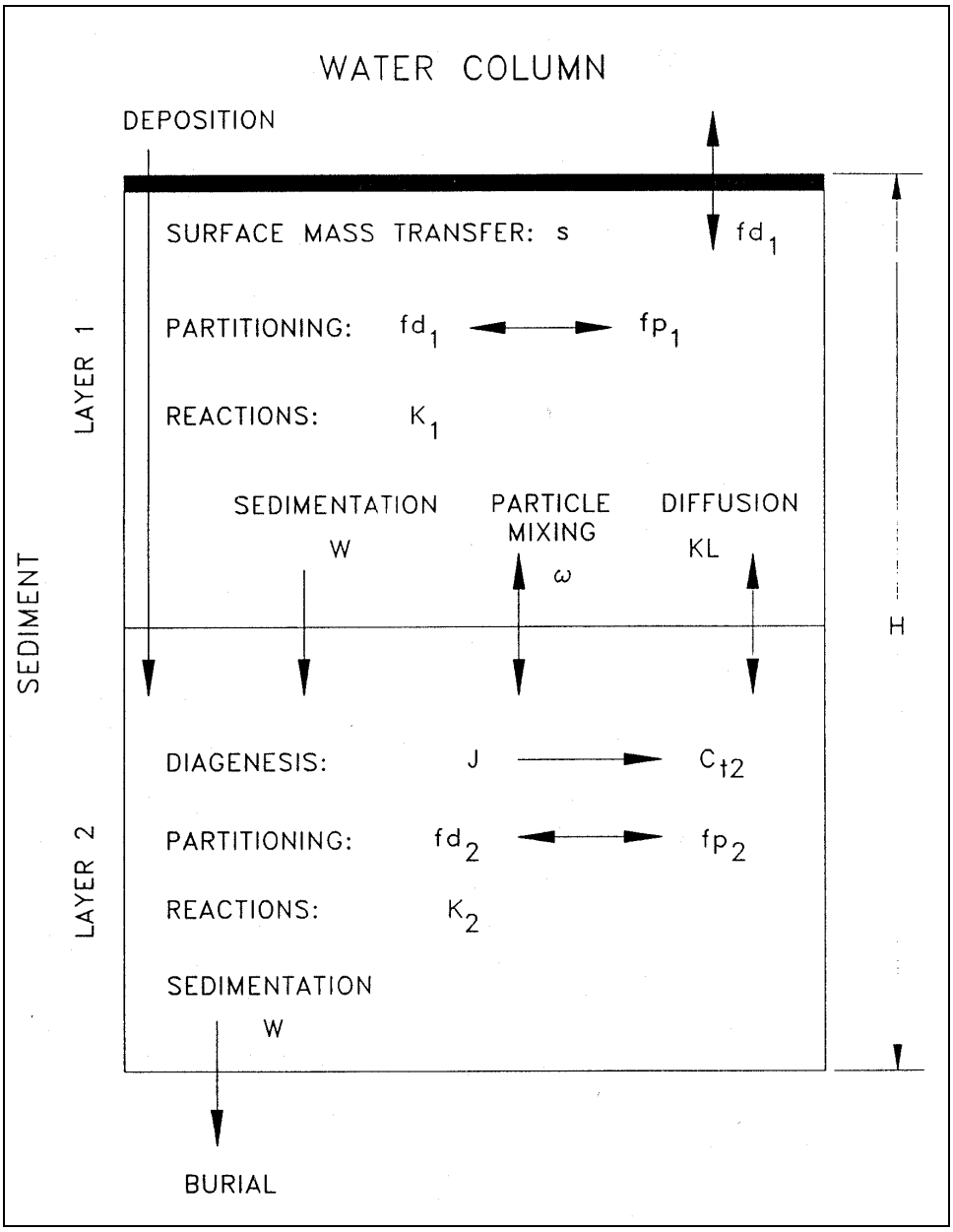

Figure 5. Sediment model elevation

The Benthos Model

Introduction

The ultimate aim of eutrophication modeling is to preserve precious living resources. Usually, the modeling process involves the simulation of living-resource parameters such as dissolved oxygen. For the "Virginia Tributary Refinements" phase of the Chesapeake Bay model activities (Cerco et al. 2002), a decision was made to initiate direct interactive simulation of three living resource groups: zooplankton, benthos, and SAV.

Benthos were included in the model because they are an important food source for crabs, finfish, and other economically and ecologically significant biota. In addition, benthos can exert a substantial influence on water quality through their filtering of overlying water. Benthos within the model were divided into two groups: deposit feeders and filter feeders (Figure 1). The deposit-feeding group represents benthos which live within bottom sediments and feed on deposited material. The filter-feeding group represents benthos which live at the sediment surface and feed by filtering overlying water.

The complete documentation of the benthos model is too extensive to repeat here. We restrict our description to the minimum required to understand the model input parameters. The primary reference for the benthos model is HydroQual (2000). This report is available on-line at http://www.chesapeakebay.net/modsc.htm. Less comprehensive descriptions may be found in Cerco and Meyers (2000) and in Meyers at al. (2000).

Deposit Feeders

The mass-balance equation for deposit feeders is:

$$\frac{d\,DF}{d\,t} = \alpha \cdot \frac{I}{m} \cdot \frac{POC \cdot Khdf}{POC + Khdf} \cdot DF - r \cdot DF - \beta \cdot DF^2 - hmr \cdot DF$$

Equation 1

in which:

DF = deposit feeder biomass (mg C m^{-2})
α = assimilation efficiency ($0 < \alpha < 1$)

m = sediment solids concentration (mg m^{-3})
I = ingestion rate (mg sediment mg^{-1} deposit feeder carbon d^{-1})
POC = sediment particulate organic carbon (mg m^{-3})
Khdf = half-saturation concentration for carbon uptake (mg m^{-3})
r = specific respiration rate (d^{-1})
β = predation rate (m^2 mg^{-1} deposit feeder C d^{-1})
hmr = mortality rate due to hypoxia (d^{-1})
t = time (d)

The assimilation efficiency and half-saturation concentration are specified individually for G1 (labile) and G2 (refractory) carbon. G3 (inert) carbon is not utilized. Particulate organic nitrogen and phosphorus are consumed along with carbon and are retained by the benthos according to stoichiometric requirements.

An inverse "Michaelis-Menton" function governs ingestion. At low carbon concentrations (POC << Khdf), ingestion is proportional to available carbon (≈I · POC). At high concentrations (POC >> Khdf), ingestion approaches a constant value (≈I · Khdf).

Effect of temperature

Ingestion, respiration, and predation all have "Arrhenius" temperature dependencies:

$$I = I_{20} \cdot \theta_I^{T-20}$$

Equation 2

in which:

I_{20} = ingestion rate at 20 ^oC (mg sediment mg^{-1} deposit feeder carbon d^{-1})
θ_I = constant that controls temperature dependence of ingestion
T = temperature (^oC)

$$r = r_{20} \cdot \theta_r^{T-20}$$

Equation 3

in which:

r_{20} = respiration rate at 20 ^oC (d^{-1})
θ_r = constant that controls temperature dependence of respiration

$$\beta = \beta_{20} \cdot \theta_\beta^{T-20}$$

Equation 4

in which:

β_{20} = predation rate at 20 °C (m^2 mg^{-1} deposit feeder C d^{-1})
θ_β = constant that controls temperature dependence of predation

Dissolved Oxygen Effects

A logistic function (Figure 2) is used to describe the effects of hypoxia on ingestion, respiration, and mortality:

$$Z = \frac{1}{1 + \exp\left(1.1 \cdot \frac{DO_{hx} - DO}{DO_{hx} - DO_{qx}}\right)}$$

Equation 5

in which:

Z = logistic function ($0 < Z < 1$)
DO = dissolved oxygen in overlying water (g m^{-3})
DO_{hx} = dissolved oxygen concentration at which value of function is one-half (g m^{-3})
DO_{qx} = dissolved oxygen concentration at which value of function is one-fourth (g m^{-3})

Ingestion is then:

$$I(DO) = I \cdot Z$$

Equation 6

in which:

I(DO) = ingestion rate corrected for oxygen effects (g sediment g^{-1} deposit feeder carbon d^{-1})

An analogous relationship describes the influence of dissolved oxygen on respiration.

Mortality due to hypoxia is:

$$hmr = \frac{\ln(1/100)}{ttd} \cdot (1 - Z)$$

Equation 7

in which:

ttd = time to death for 99% of the population (d)

The model also relates predation to dissolved oxygen concentration. Predators are assumed to vanish as dissolved oxygen approaches zero. A rectangular hyperbole describes this effect:

$$\beta(DO) = \frac{DO}{Khpred + DO} \cdot \beta$$

Equation 8

in which:

β(DO) = predation rate corrected for dissolved oxygen effects (m^2 mg^{-1} deposit feeder C d^{-1})
Khpred = dissolved oxygen concentration at which predation pressure is halved (g m^{-3})

Filter Feeders

The model allows for the specification of multiple filter-feeding groups. Each is governed by the same mass-balance equation:

$$\frac{dFF}{dt} = \alpha \cdot Fr \cdot POC \cdot FF - r \cdot FF - \beta \cdot FF^2 - hmr \cdot FF$$

Equation 9

in which:

FF = filter feeder biomass (mg C m^{-2})
α = assimilation efficiency ($0 < \alpha < 1$)
Fr = filtration rate (m^3 mg^{-1} filter feeder carbon d^{-1})
POC = particulate organic carbon in overlying water (mg m^{-3})
r = specific respiration rate (d^{-1})
β = predation rate (m^2 mg^{-1} filter feeder C d^{-1})
hmr = mortality rate due to hypoxia (d^{-1})
t = time (d)

The assimilation efficiency is specified individually for each form of particulate organic matter in the water column.

Ingestion

Filtration rate is influenced by numerous environmental factors (temperature, dissolved oxygen, suspended solids) as well as by physiology. One prime determinant of filtration rate is individual size. The developers of the benthos model (HydroQual 2000) noted that individual size was related to areal biomass; high densities of areal biomass consisted of relatively large individuals. They developed a relationship between areal density (a model state variable) and individual size (not considered in the model) and used this relationship to characterize the influence of size on filtration rate:

$$Fr(M) = Fr \cdot FF^{bf}$$

Equation 10

in which:

Fr(M) = filtration rate corrected for individual size (L mg^{-1} filter feeder carbon d^{-1})
Fr = base filtration rate (L mg^{-1} filter feeder carbon d^{-1})
bf = exponent that relates filtration rate to areal biomass density

Suspended Solids Effects. High concentrations of suspended solids can induce filter feeders to reduce their filtration rate. The effect of suspended solids on filtration rate is represented with a recast version of a relationship attributed to Powell et al. (1992). First, the potential reduction in filtration rate is computed:

$$Turbred = Max(Aturb + Bturb \cdot \log_{10}(0.001 \cdot TSS), 0)$$

Equation 11

in which:

Turbred = percent reduction in filtration ($0 < Turbred < 100$)
TSS = total suspended solids concentration in overlying water (g m^{-3})
Aturb, Bturb = parameters that relate percent reduction to solids concentration

Then a corrected filtration rate is determined:

$$Fr(M, TSS) = Fr(M) \cdot (1 - 0.01 \cdot Turbred)$$

Equation 12

in which:

Fr(M,TSS) = filtration rate corrected for effects of organism size and suspended solids concentration (m^3 mg^{-1} filter feeder carbon d^{-1})

Effects of temperature and dissolved oxygen. Filtration rate increases as a function of temperature and decreases as dissolved oxygen in the water column is depleted. The effects of temperature and dissolved oxygen are represented by relationships identical to those for deposit feeders, with appropriate parameters for filter-feeding organisms.

Respiration and Mortality

As with filtration rate, specific respiration is related to the size of an organism; as size increases, specific respiration decreases. Individual size is again related to areal biomass resulting in the relationship:

$$r = r_{20} \cdot FF^{-br}$$

Equation 13

in which:

r = specific respiration rate (d^{-1})
r_{20} = base respiration rate at 20 ^{o}C (d^{-1})
br = exponent that relates respiration rate to areal biomass density

Effects of temperature and dissolved oxygen. The effects of temperature and dissolved oxygen on respiration are represented by relationships identical to those for deposit feeders, with appropriate parameters for filter-feeding organisms.

Predation and hypoxic mortality. Predation and mortality due to hypoxia are represented by relationships identical to those for deposit feeders, with appropriate parameters for filter-feeding organisms.

Model Parameters

Parameter values for the benthos model, as implemented in the most recent Chesapeake Bay application are presented in Tables 1 (deposit feeders) and 2 (filter feeders).

Table 1
Parameters in Deposit Feeder Model

Parameter	Definition	Value	Units
I_{20}	Ingestion rate at 20 ^{o}C	175	mg sediment mg^{-1} deposit feeder carbon d^{-1}
θ_I	constant that controls temperature dependence of ingestion	1.08	
r20	respiration rate at 20 ^{o}C	0.015	d^{-1}
θ_r	constant that controls temperature dependence of respiration	1.08	
β_{20}	predation rate at 20 ^{o}C	0.0001	m^2 mg^{-1} deposit feeder C d^{-1}
θ_β	constant that controls temperature dependence of predation	1.24	
Amcn	carbon-to-nitrogen ratio	5.67	mg C mg^{-1} N
Amcp	carbon-to-phosphorus ratio	45	mg C mg^{-1} P
α_{G1}	assimilation efficiency for G1 organic matter	0.8	$0 < \alpha < 1$
α_{G2}	assimilation efficiency for G2 organic matter	0.25	$0 < \alpha < 1$
$Khdf_{G1}$	half-saturation concentration for G1 carbon uptake	10^5	mg C m^{-3}
$Khdf_{G2}$	half-saturation concentration for G2 carbon uptake	10^6	mg C m^{-3}
Khpred	dissolved oxygen concentration at which predation pressure is halved	2.25	g m^{-3}
ttd	time to death for 99% of the population	14	d
DO_{hx}	dissolved oxygen concentration at which value of function is one-half	1.75	g m^{-3}
DO_{qx}	dissolved oxygen concentration at which value of function is one-fourth	1.5	g m^{-3}

Table 2
Parameters in Filter Feeder Model

Parameter	Definition	*Corbicula fluminea* (tidal fresh)	*Rangea cuneata* (oligohaline)	*Macoma baltica* and *Mercenaria mercenaria* (mesohaline)	Units
Fr_{20}	base filtration rate at 20 ^{o}C	0.216	0.109	0.163	L mg^{-1} filter feeder carbon d^{-1}
bf	exponent that relates filtration rate to areal biomass density	0.422	0.422	0.431	
θ_f	constant that controls temperature dependence of filtration	1.08	1.08	1.08	
Aturb	parameter that relates percent reduction to solids concentration	81	81	81	
Bturb	parameter that relates percent reduction to solids concentration	24	24	24	
r_{20}	base respiration rate at 20 ^{o}C	0.026	0.026	0.026	d^{-1}
br	exponent that relates respiration rate to areal biomass density	0.119	0.119	0.119	
θ_r	constant that controls temperature dependence of respiration	1.08	1.08	1.08	
β_{20}	predation rate at 20 ^{o}C	2×10^{-5}	5×10^{-5}	10^{-6}	m^2 mg^{-1} filter feeder C d^{-1}
θ_β	constant that controls temperature dependence of predation	1.12	1.12	1.12	
DO_{hx}	dissolved oxygen concentration at which value of function is one-half	1.0	1.0	1.0	g m^{-3}

Table 2
Parameters in Filter Feeder Model

Parameter	Definition	*Corbicula fluminea* (tidal fresh)	*Rangea cuneata* (oligohaline)	*Macoma baltica* and *Mercenaria mercenaria* (mesohaline)	Units
DO_{qx}	dissolved oxygen concentration at which value of function is one-quarter	0.7	0.7	0.7	g m^{-3}
Khpred	dissolved oxygen concentration at which predation pressure is halved	1.0	1.0	1.0	g m^{-3}
ttd	time to death for 99% of the population	14	14	14	d
α_{alg}	assimilation efficiency for phytoplankton	0.8	0.8	0.8	$0 < \alpha < 1$
α_{lab}	assimilation efficiency for labile organic matter	0.8	0.8	0.8	$0 < \alpha < 1$
α_{ref}	assimilation efficiency for refractory organic	0.0	0.0	0.0	$0 < \alpha < 1$
Imax	maximum ingestion rate	0.24	0.24	0.24	d^{-1}
SFcn	carbon-to-nitrogen ratio	5.67	5.67	5.67	mg C mg^{-1} N
SFcp	carbon-to-phosphorus ratio	45	45	45	mg C mg^{-1} P

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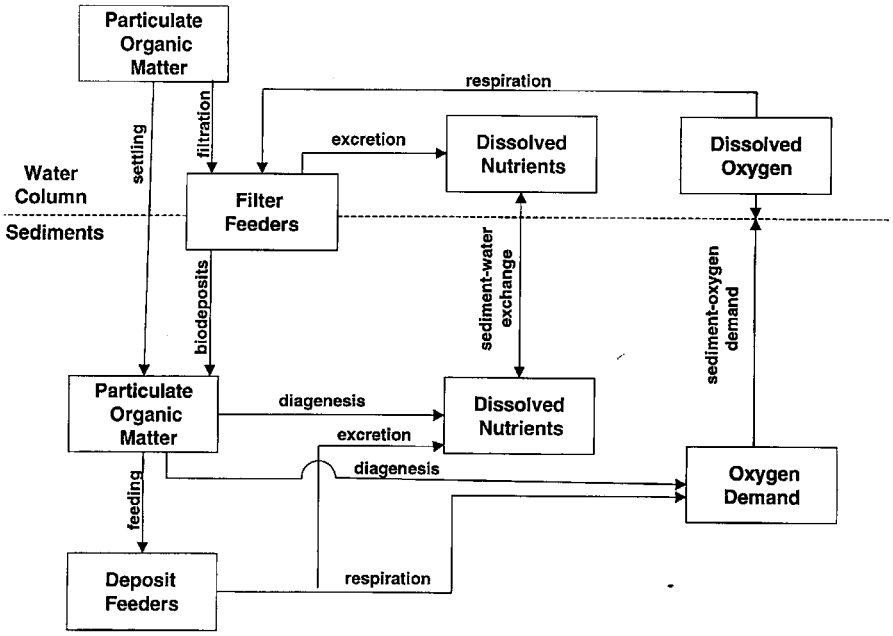

Figure 1. Benthos Model Schematic.

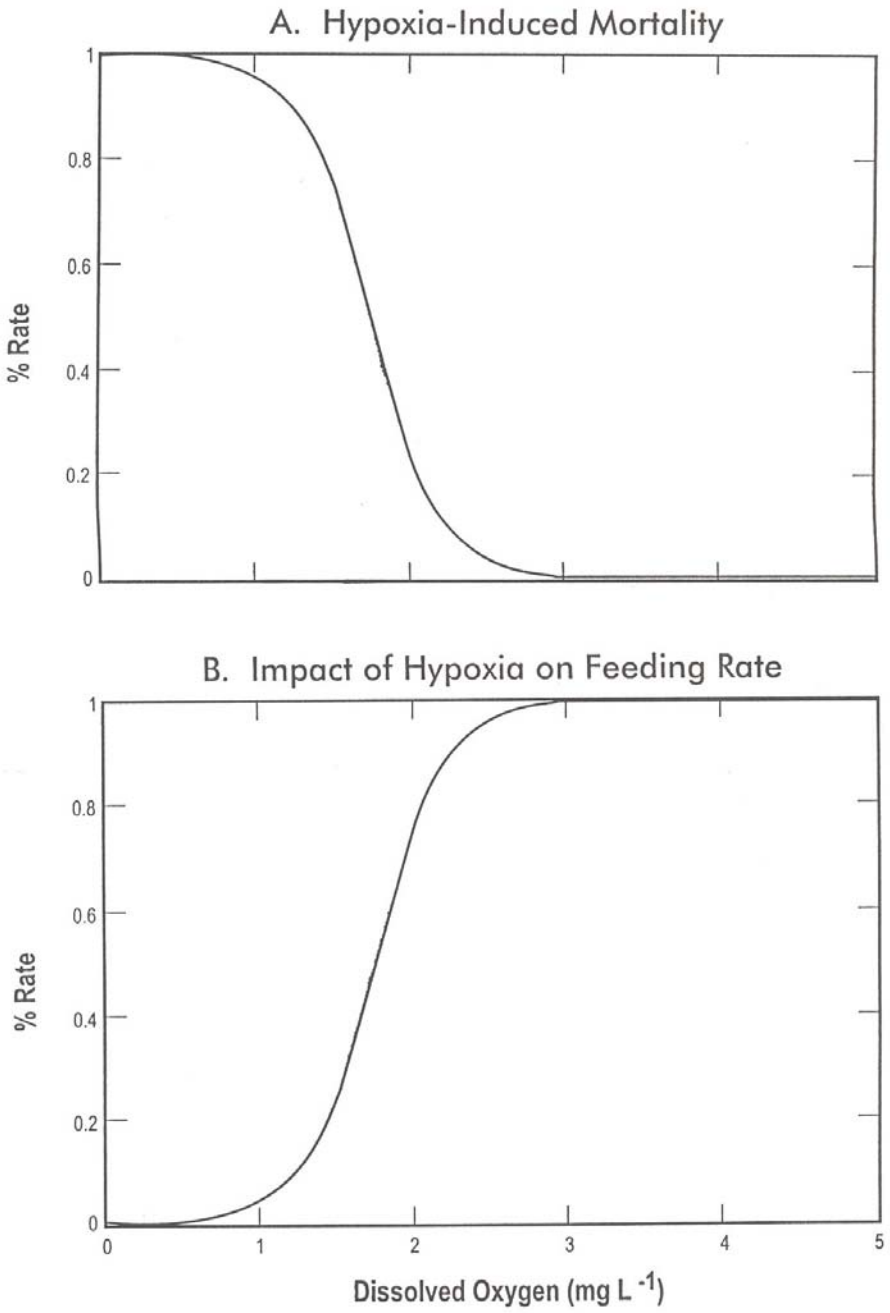

Figure 2. Effect of dissolved oxygen on mortality and feeding rate.

The Benthic Algal Model

Introduction

The benthic algal module in CE-QUAL-ICM was originally developed for the Delaware Inland Bays (Cerco and Seitzinger 1997). Production relationships and parameter values in the model were subsequently revised for consistency with revisions to phytoplankton kinetics. The benthic algal component was recalibrated during the most recent application of the Chesapeake Bay model (Cerco and Noel 2004). The primary goal of the recalibration was calculation of algal biomass comparable to measures in Chesapeake Bay and elsewhere. The formulations and parameters reported here are adapted from this most recent application.

The Benthic Algae Model

Benthic algae are considered to occupy a thin layer between the water column and benthic sediments (Figure 1). Biomass within the layer is determined by the balance of production, respiration, and losses to predation:

$$\frac{\delta B}{\delta t} = (G - BM) \cdot B - PR \qquad \textbf{(1)}$$

in which:

B = algal biomass, as carbon (g C m^{-2})
G = growth (d^{-1})
BM = basal metabolism (d^{-1})
PR = predation (g C m^{-2} d^{-1})

Formulations for production, respiration, and predation largely follow the formulations for phytoplankton ("Kinetics" chapter).

Light

The influence of light on benthic algal production is represented by a chlorophyll-specific production equation (Jassby and Platt 1976):

$$P^B = P^B m \frac{I}{\sqrt{I^2 + Ik^2}} \quad \textbf{(2)}$$

in which:

P^B = photosynthetic rate (g C g^{-1} Chl d^{-1})
$P^B m$ = maximum photosynthetic rate (g C g^{-1} Chl d^{-1})
I = irradiance (E m^{-2} d^{-1})

Parameter Ik is defined as the irradiance at which the initial slope of the production vs. irradiance relationship intersects the value of $P^B m$

$$Ik = \frac{p^B m}{\alpha} \quad \textbf{(3)}$$

in which:

α = initial slope of production vs. irradiance relationship (g C g^{-1} Chl (E m^{-2})$^{-1}$)

Chlorophyll-specific production rate is readily converted to carbon specific growth rate, for use in Equation 2, through division by the carbon-to-chlorophyll ratio:

$$G = \frac{P^B}{CChl} \quad \textbf{(4)}$$

in which:

CChl = carbon-to-chlorophyll ratio (g C g^{-1} chlorophyll a)

Light within the algal layer is attenuated by two components: solids intermingled with the algae and the algae themselves. That is:

$$Ktotal = Ksed + Kba \cdot B \quad \textbf{(5)}$$

in which:

Ktotal = sum of attenuation from sediment solids and benthic algae
Ksed = attenuation from sediment solids
Kba = attenuation from benthic algae (m^2 g^{-1} C)

Irradiance in the mat varies from the surface (no attenuation from algae) to bottom (attenuation from total algal biomass). The mean irradiance within the mat is:

$$I = \frac{Iatbot}{B} \cdot \int_0^B e^{-(Ksed + Kba \cdot B)} dB$$
$$= \frac{Iatbot \cdot e^{-Ksed}}{Kba \cdot B} \cdot [1 - e^{-Kba \cdot B}] \quad \textbf{(6)}$$

in which:

I = mean irradiance within algal mat (E m^{-2} d^{-1})
Iatbot = irradiance at bottom of water column (E m^{-2} d^{-1})

Nutrients

Carbon, nitrogen, and phosphorus are the primary nutrients required for algal growth. Benthic diatoms require silica, as well. Inorganic carbon and silica are usually available in excess and are not considered in the model. The effects of the remaining nutrients on growth are described by the formulation commonly referred to as "Michaelis-Menton kinetics":

$$f(N) = \frac{N}{KHd + N} \quad \textbf{(7)}$$

in which:

f(N) = nutrient limitation on algal production ($0 \leq f(N) \leq 1$)
N = concentration of dissolved nutrient (g m^{-3})
KHd = half-saturation constant for nutrient uptake (g m^{-3})

Due to their position at the sediment-water interface, benthic algae may utilize nutrients released from the sediments by diagenetic processes or they may remove nutrients from the water column. Since the thickness of the benthic algal layer is undefined, computation of nutrient concentration within the layer is impossible. Instead, an areal nutrient concentration that combines diagenetic nutrient flux with nutrients in the water column is computed:

$$N = Nflux \cdot \Delta t + Nwat \cdot H \quad \textbf{(8)}$$

in which:

N = areal nutrient concentration (g m^{-2})
Nflux = sediment nutrient release (g m^{-2} d^{-1})
Δt = model time step (d)
Nwat = nutrient concentration in water column (g m^{-3})
H = depth of water column (m)

Nitrogen constituents available for algal growth are ammonium plus nitrate. The preference for utilization of ammonium over nitrate is expressed with a function identical to phytoplankton (Equation 13, "Kinetics" chapter).

Dissolved phosphate is the only phosphorus constituent available for algal growth.

Temperature

Benthic algal production increases as a function of temperature until an optimum temperature or temperature range is reached. Above the optimum, production declines until a temperature lethal to the organisms is attained. Inspection of growth versus temperature data indicates a function similar to a Gaussian probability curve provides a good fit to observations:

$$\begin{aligned} f(T) &= e^{-KTg1\cdot(T-Topt)^2} \quad \text{when T} \le \text{Topt} \\ &= e^{-KTg2\cdot(Topt-T)^2} \quad \text{when T} > \text{Topt} \end{aligned} \qquad \textbf{(9)}$$

in which:

T = temperature (^oC)
Topt = optimal temperature for algal growth (^oC)
KTg1 = effect of temperature below Topt on growth ($^oC^{-2}$)
KTg2 = effect of temperature above Topt on growth ($^oC^{-2}$)

Combining Effects of Light, Nutrients, and Temperature

Phytoplankton models that consider multiple nutrients commonly invoke Leibig's "law of the minimum" so that the nutrient limitation on growth is determined by the single most limiting nutrient. This logic is not always extended to incorporate the light limitation, however. Often, the nutrient limitation is multiplied by the light limit. As an alternative, Leibig's law can be extended to include light so that growth limitation is determined by the minimum of light or one of two nutrients. Extension of Leibig's law to include light seems most rational. That is, it takes a fixed ratio of nutrients and photons to produce a unit of carbon. Production will be limited by whichever one of these is most limiting. Thus, benthic algal growth rate is expressed:

$$G = \frac{P^B m}{CChl}\cdot f(T)\cdot \text{minimum}\left(\frac{Na}{KHn+Na}, \frac{Pa}{KHp+Pa}, \frac{I}{\sqrt{I^2+Ik^2}}\right) \qquad \textbf{(10)}$$

in which:
Na = areal nitrogen concentration (g N m^{-2})
KHn = half-saturation concentration for nitrogen uptake (g N m^{-3})
Pa = areal dissolved phosphate concentration (g P m^{-2})
KHp = half-saturation concentration for phosphorus uptake (g P m^{-3})

Basal Metabolism

Basal metabolism is considered to be an exponentially increasing function of temperature:

$$BM = BMr \cdot e^{KTb \cdot (T - Tr)} \quad \textbf{(11)}$$

in which:

BMr = metabolic rate at Tr (d^{-1})
KTb = effect of temperature on metabolism ($^oC^{-1}$)
Tr = reference temperature for metabolism (^oC)

Predation

Predation is modeled by assuming predators scour a fixed area of bottom sediments per unit biomass:

$$PR = F \cdot B \cdot Z \quad \textbf{(12)}$$

F = scour rate ($m^2\ g^{-1}$ predator C day^{-1})
Z = predator biomass (g C m^{-2})

Absent an explicit model, specification of the spatial and temporal distribution of the predator population is impossible. One approach is to assume predator biomass is proportional to algal biomass, $Z = \gamma B$, in which case Equation 12 can be rewritten:

$$PR = \gamma \cdot F \cdot B^2 \quad \textbf{(13)}$$

Since neither γ nor F are known precisely, the logical approach is to combine their product into a single unknown, Phtl, determined during the model calibration procedure. Effect of temperature on predation is represented with the same formulation as the effect of temperature on respiration.

Influence of Benthic Algae on Fluxes of Dissolved Substances

In the present model, sediment-water fluxes are quantified at the interface of the algal layer and the water column. Fluxes quantified at this interface are comparable to field measurements conducted in dome-like enclosures. The benthic algae modify fluxes that would otherwise occur between water and sediments. Benthic algae may enhance, diminish, or even reverse the direction of sediment-water nutrient fluxes by intercepting diagenetically produced nutrients, by scavenging nutrients from the overlying water, and by metabolic release of internal nutrient pools. Benthic algae may enhance, diminish, or reverse the direction of sediment-water oxygen flux through photosynthetic oxygen production and through respiration.

Ammonium Flux

Diagenetic ammonium flux is enhanced by ammonium released through algal metabolism and predation on benthic algae. Diagenetic flux is diminished by uptake associated with algal production. These influences on sediment-water

ammonium flux are represented:

$$BENNH4 = DIANH4 + [(BM \cdot FNI - PN \cdot G) \cdot B + PR \cdot FNI] \cdot ANC \quad \textbf{(14)}$$

in which:

BENNH4 = sediment-water ammonium flux (g N m^{-2} d^{-1})
DIANH4 = diagenetic ammonium flux (g N m^{-2} d^{-1})
BM = benthic algal metabolism (d^{-1})
FNI = fraction of metabolic products and predation released as ammonium ($0 \leq FNI \leq 1$)
PN = nitrogen preference ($0 \leq PN \leq 1$)
PR = predation on benthic algae (g C m^{-2} d^{-1})
ANC = nitrogen-to-carbon ratio of benthic algae (g N g^{-1} C)

In the absence of benthic algae, sediment-water ammonium flux is equivalent to diagenetic ammonium flux. Net algal production causes sediment-water ammonium flux to be less than flux of diagenetically-produced ammonium. In the presence of substantial algal production, demand may exceed availability of ammonium from sediments in which case sediment-water flux is negative indicating removal of ammonium from the water column.

Nitrate Flux

Benthic algal production enhances sediment nitrate uptake when ammonium is unavailable to satisfy algal requirements:

$$BENNO3 = DIANO3 - (1 - PN) \cdot P \cdot B \cdot ANC \quad \textbf{(15)}$$

in which:

BENNO3 = sediment-water nitrate flux (g N m^{-2} d^{-1})
DIANO3 = diagenetic nitrate flux (g N m^{-2} d^{-1})

Phosphorus Fluxes

Sediment-water fluxes of dissolved phosphate and dissolved organic phosphorus are represented by relationships analogous to those for ammonium.

Dissolved Oxygen and Carbon

Oxygen demand generated by diagenetic processes is enhanced by algal metabolism and diminished by algal oxygen production. These influences on sediment oxygen demand are represented:

$$BENDO = DIADO - (BM \cdot FDO - G) \cdot AOCR \cdot B \quad \textbf{(16)}$$

in which:

BENDO = sediment oxygen demand (g O_2 m^{-2} d^{-1})
DIADO = diagenetic oxygen demand (g O_2 m^{-2} d^{-1})
FDO = fraction of metabolism represented by direct oxygen consumption
($0 \leq FDO \leq 1$)
AOCR = oxygen-to-carbon mass ratio in production and respiration (= 2.67 g O_2 g^{-1} C)

Since sediment oxygen demand is a flux into the sediments, it is a negative quantity in the model. Benthic algal production counters the influence of sediment oxygen demand. Substantial algal oxygen production can exceed the rate of oxygen consumption through sulfide oxidation and metabolism and produce oxygen release from the benthic algal layer to the water column.

To prevent oxygen consumption when none is available, algal metabolism is switched from oxygen consumption to dissolved organic carbon release as oxygen approaches zero:

$$FDO = \frac{DO}{KHrb + DO} \quad \textbf{(17)}$$

in which:

Khrb = dissolved oxygen concentration at which oxygen consumption is one-half of metabolism (g DO m^{-3})

The remainder of metabolism is released as dissolved organic carbon:

$$BENDOC = BM \cdot (1 - FDO) \cdot B \quad \textbf{(18)}$$

in which:
BENDOC = sediment-water dissolved organic carbon flux (g C m^{-2} d^{-1})

Effect of Benthic Algae on Sediment Organic Matter

Algal detritus, produced in the model through metabolism and predation, contributes to the concentration of particulate organic matter in the sediments. The contribution of benthic algae to sediment particulate organic nitrogen is the fraction of metabolism plus predation not excreted as ammonium:

$$\frac{\delta PON}{\delta t} = \frac{ANC}{Hsed} \cdot (1 - FNI) \cdot (BM \cdot B + PR) \quad \textbf{(19)}$$

in which:

PON = sediment particulate organic nitrogen concentration (g m^{-3})
Hsed = thickness of active sediment layer (m)

The contribution of benthic algae to sediment particulate organic carbon is represented:

$$\frac{\delta POC}{\delta t} = \frac{PR}{Hsed} \quad \textbf{(20)}$$

in which:

POC = sediment particulate organic carbon concentration (g m^{-3})

The contribution of benthic algae to sediment particulate organic phosphorus is described by a relationship analogous to the relationship for nitrogen. Empirical coefficients are used to distribute algal organic matter to the three sediment organic matter pools (G1, G2, G3)

Parameters in Benthic Algae Model

Parameters in the benthic algae model are summarized in Table 1.

Results from the Benthic Algal Model

Computed benthic algal biomass in Chesapeake Bay ranges up to 3 g C m^{-2}, in agreement with measures conducted in a variety of systems (Table 2). The highest densities of computed benthic algae are found in shallow water near the mouths of the lower western tributaries, along the lower eastern shore, and in eastern embayments (Figure 2). Lesser densities occur in tidal fresh waters and in other shoal areas. The primary determinant of algal density is light. Algal biomass shows an inverse relationship to optical depth (total depth × light attenuation) at the sediment-water interface (Figure 3). No algae are computed above optical depth ≈ 5.

Observations collected in the Delaware Inland Bays (Cerco and Seitzinger 1997) indicated benthic sediments, incubated in the dark, released ammonium and phosphate (Figure 4). Activity of benthic algae diminished nutrient release under illumination. Ammonium and phosphate releases were eliminated when irradiance attained ≈ 150 μE m^{-2} s^{-1}. The sediments consumed oxygen in the dark. Activity of benthic algae induced oxygen production at the sediment-water interface when irradiance attained ≈ 150 μE m^{-2} s^{-1}. Sediment-water nitrate fluxes were small and showed no influence of irradiance.

We examined the effect of light on computed sediment-water fluxes by selecting a model segment rich in benthic algae. Biomass varied from 1 g C m^{-2} in winter to 3 g C m^{-2} in summer. Light at the sediment surface and sediment-water fluxes were recorded at hourly intervals over a year. Mean and range of modeled fluxes were computed for 60 μE m^{-2} s^{-1} increments of irradiance. Results were similar to the measures collected in the Delaware Inland Bays. Sediments released ammonium, nitrate, and phosphate in the dark (Figures 5 - 7). These nutrients were instead stripped from the water column at iradiance of 100 to 200 μE m^{-2} s^{-1}. Sediment consumption of oxygen, in the dark, became oxygen production as irradiance exceeded 150 μE m^{-2} s^{-1} (Figure 8). For any irradiance level, a good deal of scatter was apparent in the computed fluxes. We noted that flux depended not only on incident light but on trends in algal biomass. When biomass was trending up, nutrient uptake and oxygen release at a fixed irradiance

level were enhanced. When biomass was trending down, nutrient uptake and oxygen release at a fixed irradiance level were diminished. We concluded that the model, as presently calibrated, represents benthic algal biomass, compared to reported values, and activity, compared to reported sediment-water fluxes.

Table 1
Parameters in Benthic Algae Model

Symbol	Definition	Value	Units
ANC	nitrogen-to-carbon ratio of algae	0.167	g N g^{-1} C
APC	phosphorus-to-carbon ratio of algae	0.0167	g P g^{-1} C
BMr	basal metabolic rate of algae at reference temperature Tr	0.02	d^{-1}
CChl	carbon-to-chlorophyll ratio of algae	100	g C mg^{-1} chl
FNI	fraction of inorganic nitrogen produced by metabolism and predation	0.0	$0 \leq FNI \leq 1$
FPI	fraction of dissolved inorganic phosphorus produced by metabolism and predation	0.0	$0 \leq FPI \leq 1$
FRCPHB	fraction of particulate organic carbon distributed to sediment pools	0.65 G1 0.30 G2 0.05 G3	$0 \leq FRCPHB \leq 1$
FRNPHB	fraction of particulate organic nitrogen distributed to sediment pools	0.65 G1 0.30 G2 0.05 G3	$0 \leq FRNPHB \leq 1$
FRPPHB	fraction of particulate organic phosphorus distributed to sediment pools	0.65 G1 0.255 G2 0.095 G3	$0 \leq FPDP \leq 1$
Kba	light attenuation coefficient for benthic algae	0.2	m^2 g^{-1} C
KHn	half-saturation concentration for nitrogen uptake by algae	0.01	g N m^{-2}
KHp	half-saturation concentration for phosphorus uptake by algae	0.001	g Pm^{-2}
KHrb	half-saturation concentration for respiration	0.5	g DO m^{-3}
Ksed	light attenuation coefficient for sediments	0.5	
KTb	effect of temperature on basal metabolism of algae	0.032	$^oC^{-1}$
KTg1	effect of temperature below Tm on growth of algae	0.003	$^oC^{-2}$
KTg2	effect of temperature above Tm on growth of algae	0.01	$^oC^{-2}$
Phtl	predation rate on algae	0.1	m^2 g^{-1} C d^{-1}
PBm	production rate of algae under optimal conditions	300	g C g^{-1} Chl d^{-1}
Topt	optimal temperature for growth of algae	25	^oC
Tr	reference temperature for metabolism	20	^oC
α	initial slope of production vs. irradiance relationship	8.0	g C g^{-1} Chl $(E\ m^{-2})^{-1}$

Table 2
Reported Benthic Algal Biomass

Biomass, g C m^{-2}	System	Citation	Comments
4	Delaware Inland Bays	Cerco and Seitzinger (1997)	Computed annual average.
2.1	Goodwin Islands, York River mouth	Buzzelli (1998)	Mean of 108 observations. Converted from mg Chl a m-2 using C:Chl ratio of 50 (Gould and Gallagher 1990).
2 to 4	North Inlet SC	Pinckney and Zingmark (1993)	Range over a year. Converted from mg Chl a m^{-2} using C:Chl ratio of 50 (Gould and Gallagher 1990).
1.6	Ems-Dollard Estuary	Admiraal et al. (1983)	Converted from cells cm^{-2} using 1 g C m^{-2} = 1.25 x 10^6 cells cm^{-2} found in text.
0.4 to 7.2	Laholm Bay	Sundbäck (1986)	Range over a year observed at 14 to 16 m. Converted from cells cm^{-2} as per Admiraal et al. (1983).
2.2 to 15	Savin Hill Cove, near Boston Harbor	Gould and Gallagher (1990)	Report C:Chl of 18.7 to 60.4.

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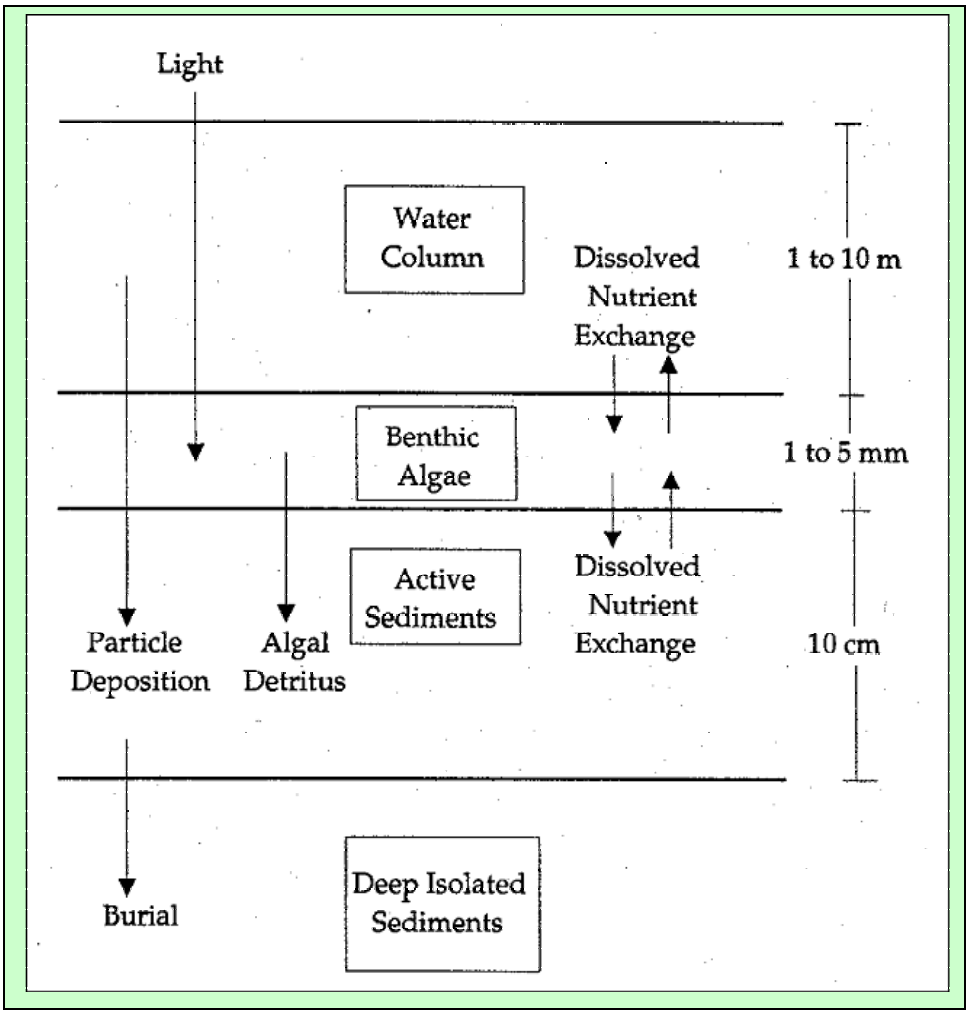

Figure 1. Benthic Algae Model Schematic

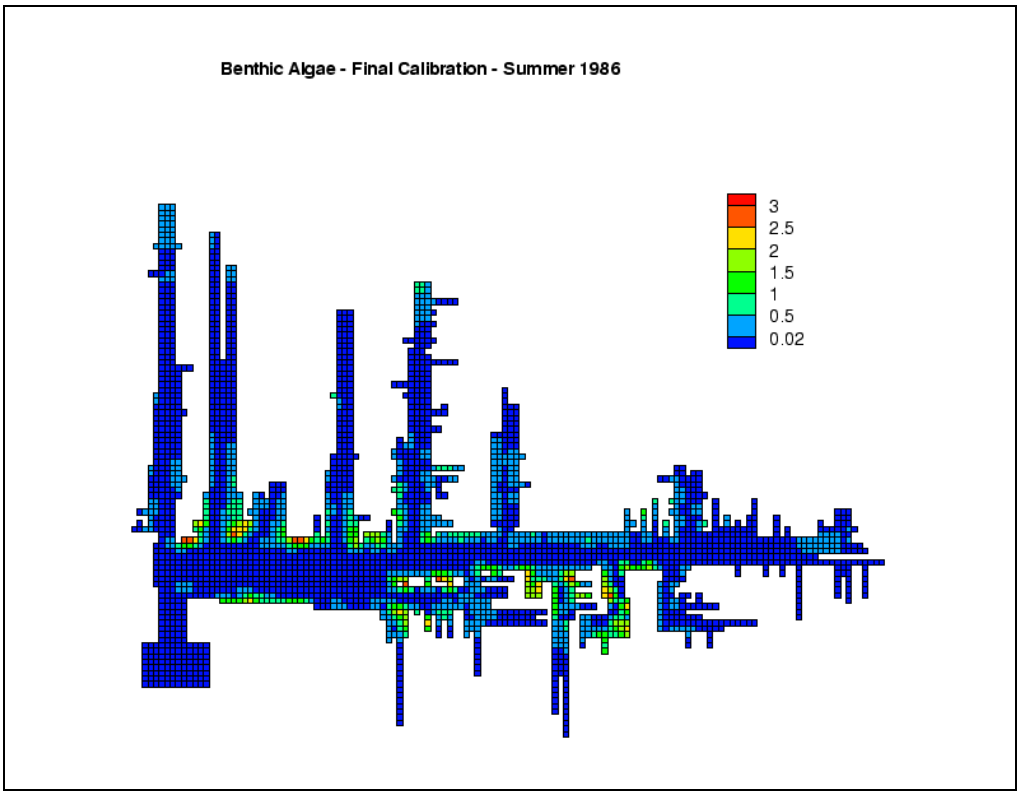

Figure 2. Computed summer-average benthic algal biomass in Chesapeake Bay, 1986.

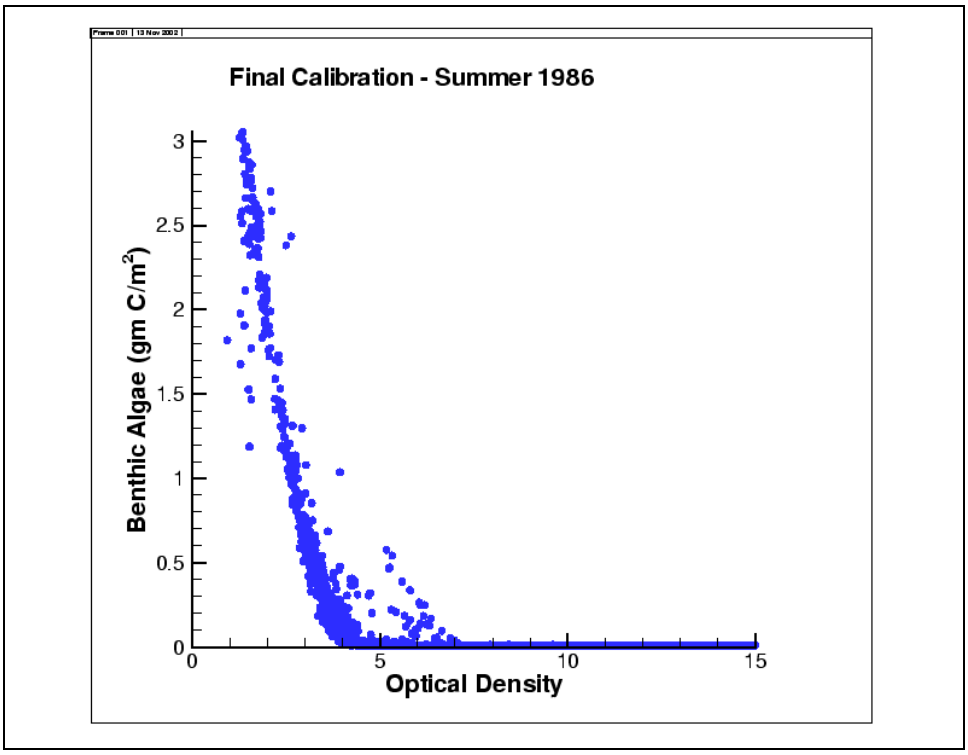

Figure 3. Summer-average benthic algal biomass versus optical density.

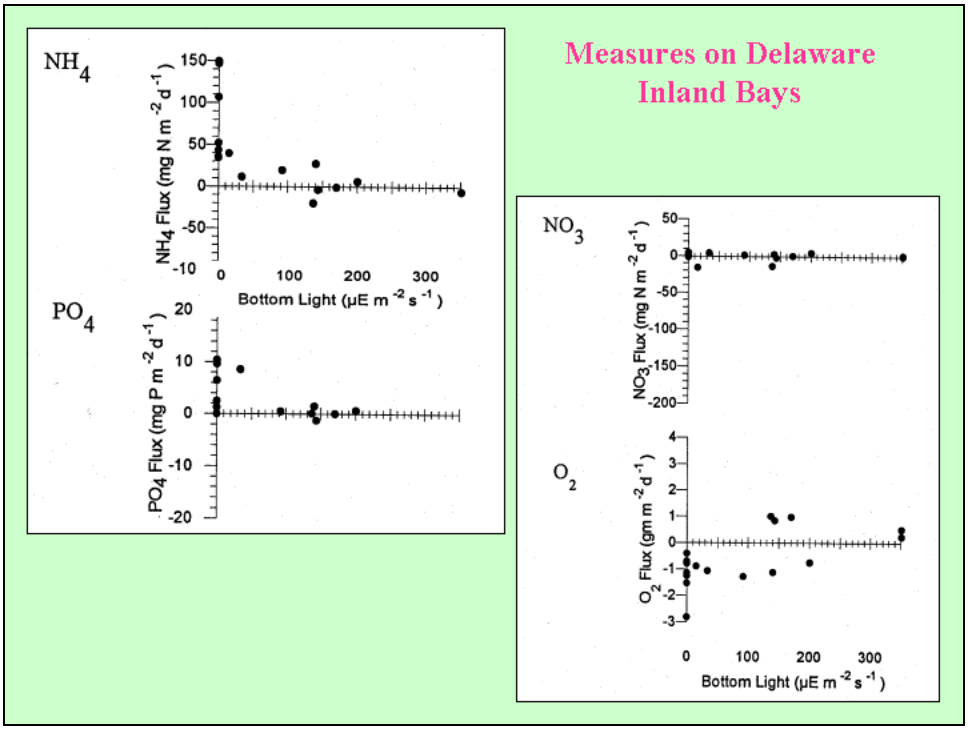

Figure 4. Sediment-water nutrient and oxygen flux observed in Delaware Inland Bays.

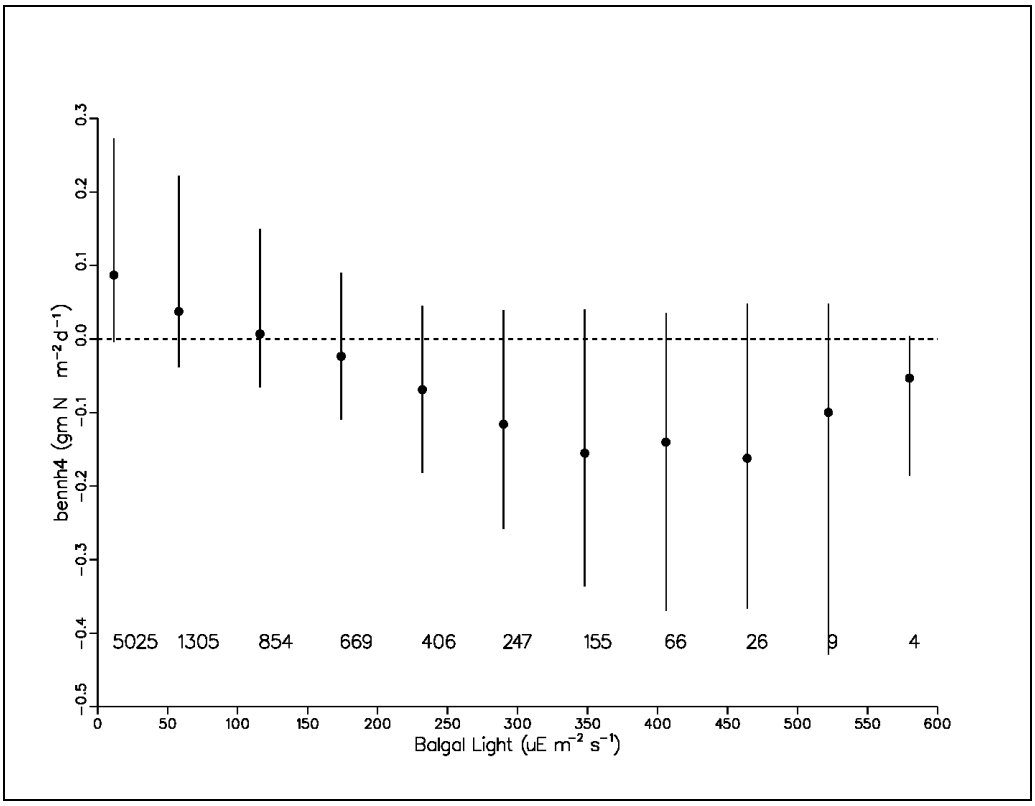

Figure 5. Computed (mean and range) sediment-water ammonium flux as a function of irradiance at the sediment-water interface. Benthic algal biomass 1 to 3 g C m^{-2}. Positive fluxes are from sediments to the water column. Number of hourly samples indicated for each irradiance increment.

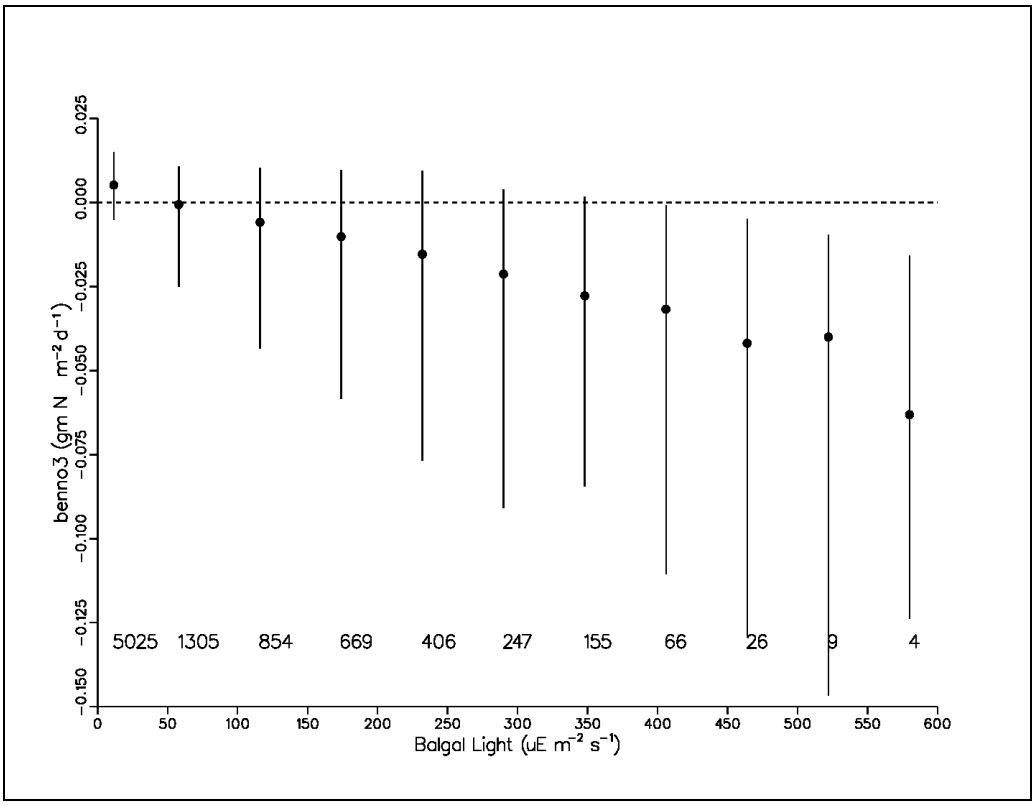

Figure 6. Computed (mean and range) sediment-water nitrate flux as a function of irradiance at the sediment-water interface. Benthic algal biomass 1 to 3 g C m^{-2}. Positive fluxes are from sediments to the water column. Number of hourly samples indicated for each irradiance increment.

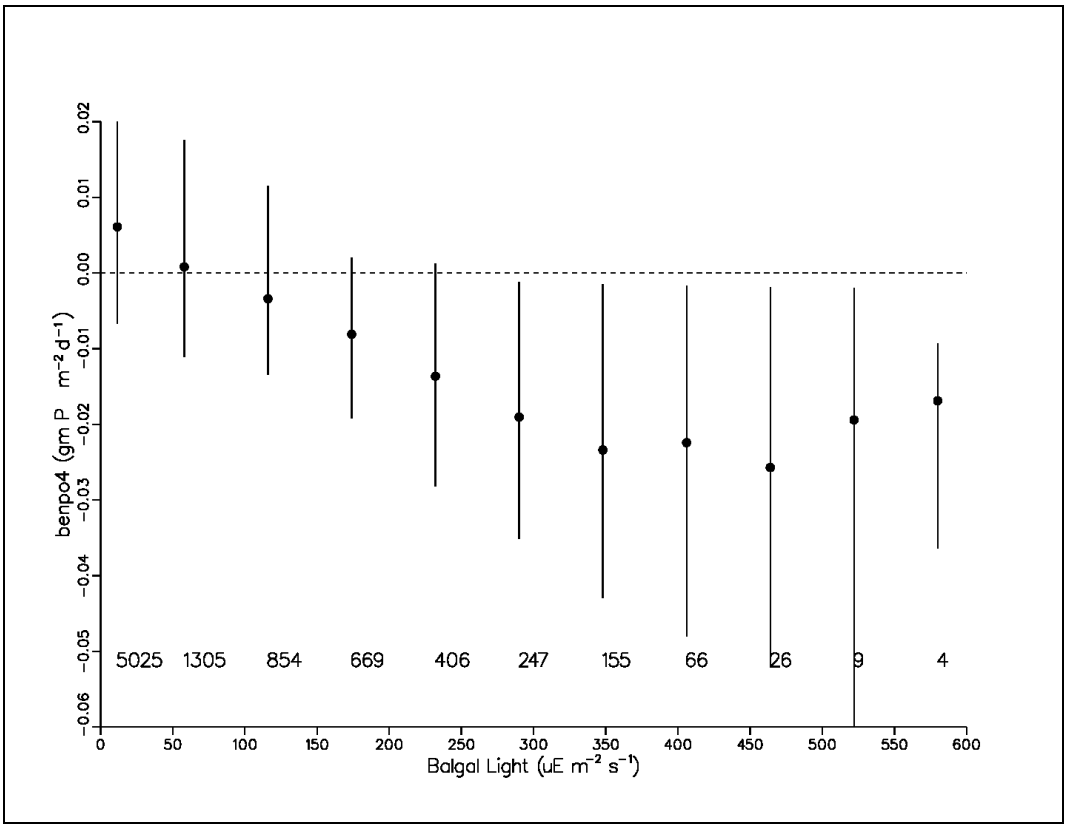

Figure 7. Computed (mean and range) sediment-water phosphate flux as a function of irradiance at the sediment-water interface. Benthic algal biomass 1 to 3 g C m^{-2}. Positive fluxes are from sediments to the water column. Number of hourly samples indicated for each irradiance increment.

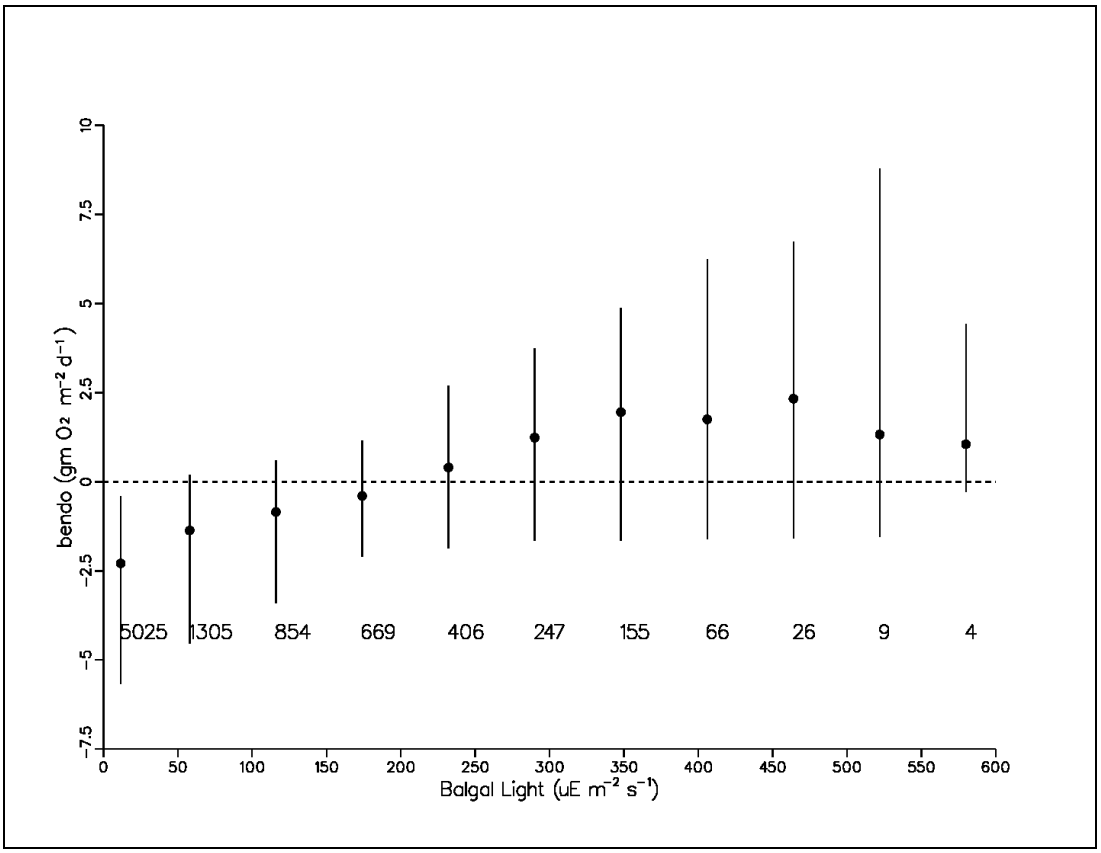

Figure 8. Computed (mean and range) sediment-water dissolved oxygen flux as a function of irradiance at the sediment-water interface. Benthic algal biomass 1 to 3 g C m^{-2}. Positive fluxes are from sediments to the water column. Number of hourly samples indicated for each irradiance increment

Input to the Sediment Diagenesis Model

The Benthic Flux Input File takes two formats, depending on the specification of SEDC and BFC in the Control File. If SEDC = "ON" the file contains input to the predictive sediment submodel. If BFC = "ON" the file contains user-specified benthic fluxes. If both parameters are "OFF" the file is not opened.

Input to the predictive model is addressed first. The input file was assembled by multiple individuals at various times and is constructed with a multitude of formats and mixed units.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe sediment submodel input deck

Three title lines are required to describe the sediment input deck. These are not read as variables but are skipped by a FORMAT statement.

Example

```
SENS50 Mar 23, 2001  No fresh/salt differences
Increase WSS, WSSNET mostly in tribs.     3/27/01
No enhanced algal settling in turb max.
```

Miscellaneous Parameters

Following a title line, the thickness of the active sediment layer and parameter INTSED are specified. The G3 component of sediment organic matter takes decades to come to steady state. Estimates of steady-state G3 carbon, nitrogen, and phosphorus are substituted for computed G3 organic mater in the initial conditions output file if INTSEDC = 1. If INTSEDC = 0, no estimate is provided. The format for these parameters is (8X,F8.0,I8). Sediment temperature is predicted based on the diffusion of heat between the water column and sediments. The diffusion coefficient is next input with format (8F10.0).

Empirical evidence indicates differences between fresh and saltwater phosphate sorption capacity and nitrification/denitrification rates. SALTSW and

SALTND are used to indicate the salinity at which differing phosphate sorption and nitrification/denitrification rates are employed. The format for these inputs is (8F10.0)

Field	Name	Value	Description
1	HSED	Real	Thickness of active sediment layer (cm)
2	INTSED	Integer	A flag to provide steady-state integration of G3 organic matter
1	DIFFT	Real	Thermal diffusion coefficient ($cm^2\ s^{-1}$)
1	SALTSW	Real	Freshwater phosphate absorption coefficients are used below this salinity (ppt)
2	SALTNT	Real	Freshwater nitrification/denitrification rates are used below this salinity (ppt)

Example

```
          HSED  INTSED
          10.0       1
0.0018                                   difft
  1.00       1.0                      saltsw,SALTND
```

Algal Organic Matter Splits

Upon deposition, organic matter associated with phytoplankton and benthic algae must be mapped into the three sediment G classes. The sum of the splits for each substance and algal group must equal unity. The format of these inputs is (8F10.0)

Field	Name	Value	Description
1	FRPPH1(1)	Real	G1 fraction of algal group 1 phosphorus
2	FRPPH1(2)	Real	G2 fraction of algal group 1 phosphorus
3	FRPPH1(3)	Real	G3 fraction of algal group 1 phosphorus
1	FRPPH2(1)	Real	G1 fraction of algal group 2 phosphorus
2	FRPPH2(2)	Real	G2 fraction of algal group 2 phosphorus
3	FRPPH2(3)	Real	G3 fraction of algal group 2 phosphorus
1	FRPPH3(1)	Real	G1 fraction of algal group 3 phosphorus
2	FRPPH3(2)	Real	G2 fraction of algal group 3 phosphorus
3	FRPPH3(3)	Real	G3 fraction of algal group 3 phosphorus
1	FRPPHB(1)	Real	G1 fraction of benthic algal phosphorus
2	FRPPHB(2)	Real	G2 fraction of benthic algal phosphorus
3	FRPPHB(3)	Real	G3 fraction of benthic algal phosphorus
1	FRNPH1(1)	Real	G1 fraction of algal group 1 nitrogen
2	FRNPH1(2)	Real	G2 fraction of algal group 1 nitrogen
3	FRNPH1(3)	Real	G3 fraction of algal group 1 nitrogen
1	FRNPH2(1)	Real	G1 fraction of algal group 2 nitrogen
2	FRNPH2(2)	Real	G2 fraction of algal group 2 nitrogen
3	FRNPH2(3)	Real	G3 fraction of algal group 2 nitrogen
1	FRNPH3(1)	Real	G1 fraction of algal group 3 nitrogen
2	FRNPH3(2)	Real	G2 fraction of algal group 3 nitrogen
3	FRNPH3(3)	Real	G3 fraction of algal group 3 nitrogen

1	FRNPHB(1)	Real	G1 fraction of benthic algal nitrogen
2	FRNPHB(2)	Real	G2 fraction of benthic algal nitrogen
3	FRNPHB(3)	Real	G3 fraction of benthic algal nitrogen
1	FRCPH1(1)	Real	G1 fraction of algal group 1 carbon
2	FRCPH1(2)	Real	G2 fraction of algal group 1 carbon
3	FRCPH1(3)	Real	G3 fraction of algal group 1 carbon
1	FRCPH2(1)	Real	G1 fraction of algal group 2 carbon
2	FRCPH2(2)	Real	G2 fraction of algal group 2 carbon
3	FRCPH2(3)	Real	G3 fraction of algal group 2 carbon
1	FRCPH3(1)	Real	G1 fraction of algal group 3 carbon
2	FRCPH3(2)	Real	G2 fraction of algal group 3 carbon
3	FRCPH3(3)	Real	G3 fraction of algal group 3 carbon
1	FRCPHB(1)	Real	G1 fraction of benthic algal carbon
2	FRCPHB(2)	Real	G2 fraction of benthic algal carbon
3	FRCPHB(3)	Real	G3 fraction of benthic algal carbon

Example

```
0.65     0.255     0.095              FRPPH1
0.65     0.255     0.095              FRPPH2
0.65     0.255     0.095              FRPPH3
0.65     0.255     0.095              FRPPHB
0.65     0.300     0.050              FRNPH1
0.65     0.300     0.050              FRNPH2
0.65     0.300     0.050              FRNPH3
0.65     0.300     0.050              FRNPHB
0.65     0.255     0.095              FRCPH1
0.65     0.255     0.095              FRCPH2
0.65     0.255     0.095              FRCPH3
0.65     0.255     0.095              FRCPHB
```

Diagenesis Rates

G1, G2, G3 classes of organic matter undergo diagenesis (decay) at different rates. Diagenesis is enhanced at higher temperatures, diminished at lower temperatures. Details of the formulation of the diagenesis reaction are presented in the "Sediment-Water Interactions" chapter. The format for these inputs is (8F10.0).

Field	Name	Value	Description
1	KPDIAG(1)	Real	Diagenesis rate of G1 phosphorus at 20 ^{o}C (d^{-1})
2	DPTHTA(1)	Real	Effect of temperature on G1 phosphorus diagenesis
3	KPDIAG(2)	Real	Diagenesis rate of G2 phosphorus at 20 ^{o}C (d^{-1})
4	DPTHTA(2)	Real	Effect of temperature on G2 phosphorus diagenesis
5	KPDIAG(3)	Real	Diagenesis rate of G3 phosphorus at 20 ^{o}C (d^{-1})
6	DPTHTA(3)	Real	Effect of temperature on G3 phosphorus diagenesis
1	KNDIAG(1)	Real	Diagenesis rate of G1 nitrogen at 20 ^{o}C (d^{-1})

2	DNTHTA(1)	Real	Effect of temperature on G1 nitrogen diagenesis
3	KNDIAG(2)	Real	Diagenesis rate of G2 nitrogen at 20 ^{o}C (d^{-1})
4	DNTHTA(2)	Real	Effect of temperature on G2 nitrogen diagenesis
5	KNDIAG(3)	Real	Diagenesis rate of G3 nitrogen at 20 ^{o}C (d^{-1})
6	DNTHTA(3)	Real	Effect of temperature on G3 nitrogen diagenesis
1	KCDIAG(1)	Real	Diagenesis rate of G1 carbon at 20 ^{o}C (d^{-1})
2	DCTHTA(1)	Real	Effect of temperature on G1 carbon diagenesis
3	KCDIAG(2)	Real	Diagenesis rate of G2 carbon at 20 ^{o}C (d^{-1})
4	DCTHTA(2)	Real	Effect of temperature on G2 carbon diagenesis
5	KCDIAG(3)	Real	Diagenesis rate of G3 carbon at 20 ^{o}C (d^{-1})
6	DCTHTA(3)	Real	Effect of temperature on G3 carbon diagenesis
1	KSI	Real	Particulate biogenic silica dissolution rate at 20 ^{o}C (d^{-1})
2	THTASI	Real	Effect of temperature on silica dissolution

Example

```
0.035      1.10    0.0018     1.150   0.00000      1.17    pop1 diag
0.035      1.10    0.0018     1.150   0.00000      1.17    pon1 diag
0.035      1.10    0.0018     1.150   0.00000      1.17    poc1 diag
0.500      1.10                                            pos diag
```

Additional Parameters

Specification of inorganic solids concentration in the sediments is required to compute concentration and flux of substances sorbed to these solids. Both particle mixing and diffusion of dissolved substances are affected by temperature. Formulation of the temperature effect is presented in the sediment model documentation. The convention for these inputs includes a blank line, a header line, and parameter specification (//8X,8F8.1).

Field	Name	Value	Description
1	M1	Real	Solids concentration in sediment layer 1 (kg L^{-1})
2	M1	Real	Solids concentration in sediment layer 1 (kg L^{-1})
3	THTADP	Real	Effect of temperature on particle mixing rate

4	THTADD	Real	Effect of temperature on porewater diffusion coefficient

Example

```
  m1      m2  thtaDp  thtaDd
 0.5     0.5   1.117    1.08
```

Diagenesis Parameters

The parameters for the diagenesis model are entered next. These parameters should not be altered by the casual user. The reader is referred to the "Sediment-Water Interactions" chapter and to the documentation of the sediment model for details on parameter definition and evaluation. The convention for these inputs includes a blank line, a header line, and parameter specification (//8X,8F8.1).

Computed sediment silica releases were much less than observed in the original model application. We theorized the problem was lack of particulate biogenic silica loading from the watershed. In the absence of loading information, the option to increment modeled silica diagenesis through parameter JSIDETR was added.

Particle mixing within the sediments is strongly influenced by bioturbation. Bioturbation depends on the abundance and activity of benthic infauna. Deposit feeders were not modeled in the original formulations. Consequently, particle mixing was related to dissolved oxygen. The principle was that low dissolved oxygen would stress the benthic infauna and reduce bioturbation. At the time of this writing, the original formulations are still active despite the addition of deposit feeders to the model suite.

Field	Name	Value	Description
1	KAPPNH4F	Real	Freshwater nitrification reaction velocity at 20^o C (m d^{-1})
2	KAPPNH4S	Real	Saltwater nitrification reaction velocity at 20^o C (m d^{-1})
3	PIENH4	Real	Partition coefficient between dissolved and sorbed ammonium (L kg^{-1})
4	THTANH4	Real	Effect of temperature on nitrification rate
5	KMNH4	Real	Half-saturation concentration of ammonium in nitrification reaction (mg N m^{-3})
6	KMNH4O2	Real	Half-saturation concentration of dissolved oxygen in nitrification reaction (g O_2 m^{-3})
1	KAPPNO3F	Real	Freshwater denitrification reaction velocity in sediment layer 1 at 20^o C (m d^{-1})

2	KAPPNO3S	Real	Saltwater denitrification reaction velocity in sediment layer 1 at 20^o C (m d^{-1})
3	K2NO3	Real	Denitrification reaction velocity in sediment layer 1 at 20^o C (m d^{-1})
4	THTANO3	Real	Effect of temperature on denitification rate
1	KAPPD1	Real	Dissolved sulfide reaction velocity at 20^o C (m d^{-1})
2	KAPPP1	Real	Particulate sulfide reaction velocity at 20^o C (m d^{-1})
3	PIE1S	Real	Partition coefficient between dissolved and sorbed sulfide in layer 1 (L kg^{-1})
4	PIE2S	Real	Partition coefficient between dissolved and sorbed sulfide in layer 2 (L kg^{-1})
5	THTAPD1	Real	Effect of temperature on sulfide oxidation rate
6	KMHSO2	Real	Effect of dissolved oxygen on sulfide oxidation (g O_2 m^{-3})
1	CSISAT	Real	Saturation concentration of porewater silica (mg Si m^{-3})
2	PIE1SI	Real	Incremental partition coefficient for silica in sediment layer 1
3	PIE2SI	Real	Partition coefficient between dissolved and sorbed silica in layer 2 (L kg^{-1})
4	KMPSI	Real	Half-saturation concentration of dissolved silica in dissolution reaction (mg Si m^{-3})
1	O2CRITSI	Real	Effect of dissolved oxygen on silica sorption (g O_2 m^{-3})
2	JSIDETR	Real	Distributed source of sediment biogenic silica (mg Si m^{-2} d^{-1})
1	PI1PO4F	Real	Incremental partition coefficient for phosphate in sediment layer 1, freshwater
2	PI1PO4S	Real	Incremental partition coefficient for phosphate in sediment layer 1, saltwater
3	PI2PO4	Real	Partition coefficient between dissolved and sorbed phosphate in layer 2 (L kg^{-1})
4	O2CRIT	Real	Effect of dissolved oxygen on phosphate sorption (g O_2 m^{-3})
5	KMO2DP	Real	Half-saturation concentration for dissolved oxygen effect on particle mixing (g O_2 m^{-3})
1	TEMPBNTH	Real	Temperature at which benthic stress is reset to zero (C^o)
2	KBNTSTR	Real	First-order rate at which benthic stress subsides (d^{-1})
3	KLBNTH	Real	Ratio of bioirrigation to bioturbation
4	DPMIN	Real	Minimum particle mixing coefficient (m^2 d^{-1})

1	KAPPCH4	Real	Methane oxidation reaction velocity at 20° C (m d^{-1})
2	THTACH4	Real	Effect of temperature on methane oxidation
3	KMCH4O2	Real	Dissolved oxygen concentration at which methane oxidation is halved (g O_2 m^{-3})
4	KMSO4	Real	Sulfate concentration below which half of organic matter oxidation is via methane formation (g O_2-equivalents m^{-3})

Example

```
 kapnh4f KAPNH4s  pienh4 thtanh4   kmnh4 kmnh4o2
   0.140   0.140     1.0    1.08   1500.    1.00

 kapno3f KAPNO3s   k2no3 thtano3
     0.3   0.125    0.25    1.08

  kappd1  kappp1   pie1s   pie2s thtapd1 kmmhso2
     0.2     0.4    100.    100.    1.08     4.0

  csisat  pie1si  pie2si   kmpsi
  40000.    10.0    100. 5.0E+07

O2CRITSI JSIDETR
     1.0     0.0                       Jsidetr was 100.

 pi1po4f PI1PO4S  pi2po4  o2crit  kmo2Dp
    150.    150.     50.      2.     4.0

tempbnth kbntstr  KLBNTH   DPMIN
    10.0    0.03    00.0  3.0E-6

 kappch4 thtach4 kmch4o2   kmso4
     0.2    1.08     0.2     0.1
```

Deposit-Feeder Parameters

Parameters for the deposit feeders, described in "The Benthos Model," are input through the Benthic Flux Input file. These parameters must be listed even if the deposit feeders are not activated. The convention for these inputs includes a blank line, a header line, and parameter specification (//8X,8F8.1).

Field	Name	Value	Description
1	XKMI0	Real	Dissolved oxygen concentration at which ingestion is halved, not used in present code (g O_2 m^{-3})
2	I0	Real	Ingestion rate at 20 °C (mg sediment mg^{-1} deposit feeder carbon d^{-1})
3	THTAI0	Real	Constant that controls temperature dependence of ingestion
4	R	Real	Respiration rate at at 20 °C ($d^{-}1$)
5	THTAR	Real	Constant that controls temperature dependence of respiration

6	BETA	Real	Predation rate at 20 ^{o}C (m^2 mg^{-1} deposit feeder carbon d^{-1})
7	THBETA	Real	Constant that controls temperature dependence of predation
1	AMCN	Real	Carbon-to-nitrogen ratio (mg C mg^{-1} N)
2	AMCP	Real	Carbon-to-phosphorus ratio (mg C mg^{-1} P)
3	A	Real	Assimilation efficiency for G1 organic matter ($0 \leq A \leq 1$)
4	AA	Real	Assimilation efficiency for G2 organic matter ($0 \leq AA \leq 1$)
5	XKMG1	Real	Half-saturation concentration for G1 carbon uptake (mg C m^{-3})
6	XKMG2	Real	Half-saturation concentration for G2 carbon uptake (mg C m^{-3})
1	XKBO2	Real	Dissolved oxygen concentration at which predation pressure is halved (g m^{-3})
2	TDD	Real	Time to death for 99% of the population (d)
3	DOLOW	Real	Not utilized
4	DFDOH	Real	Dissolved oxygen concentration at which value of logistic function is one-half (g m^{-3})
5	DFDOQ	Real	Dissolved oxygen concentration at which value of logistic function is one-quarter (g m^{-3})

Example

```
           xkmi0      i0  thtai0       r   thtar    beta  thbeta
DEPF1     1.0000   175.0    1.08   0.015   1.080  1.0e-4    1.24

            amcn    amcp       a      aa   xkmg1   xkmg2
DEPF2     5.6700   45.00    0.80    0.25  1.0e+5  1.0e+6

           xkbo2     tdd   dolow   DFDOh   DFDOq
DEPF3     2.2500   14.00    1.00    1.75    1.50
```

Benthic Algae Parameters

Parameters for benthic algae are input through the Benthic Flux Input file. These parameters must be listed even if benthic algae are not activated. The convention for these inputs includes a blank line, a header line, and parameter specification. The format for the character input is (//13X,A3). The format for all other inputs is (//8X,8F8.1). To activate benthic algae, parameter BALCG must be specified as ‘ ON’ in uppercase characters.

Field	**Name**	**Value**	**Description**
1	BALGC	Character	BALCG = ‘ ON’ activates benthic algae
1	PMB	Real	Production rate of algae under optimal conditions (g C g^{-1} Chl d^{-1})
2	ANCB	Real	Nitrogen-to-carbon ratio (g N g^{-1} C)

3	APCB	Real	Phosphorus-to-carbon ratio (g P g^{-1} C)
4	KTGB1	Real	Effect of sub-optimal temperature on growth of benthic algae ($^oC^{-2}$)
5	KTGB2	Real	Effect of super-optimal temperature on growth of benthic algae ($^oC^{-2}$)
6	TMB	Real	Optimal temperature for growth of benthic algae (^{o}C)
1	ALPHB	Real	Initial slope of production vs. irradiance relationship (g C g^{-1} Chl (E m^{-2})$^{-1}$)
2	CCHLB	Real	Carbon-to-chlorophyll ratio (g C g^{-1} Chl)
3	KESED	Real	Light attenuation coefficient for sediments
4	KEBALG	Real	Light attenuation coefficient for benthic algae (m^2 g^{-1} C)
5	KHNB	Real	Half-saturation concentration for nitrogen uptake (g N m^{-2})
6	KHPB	Real	Half-saturation concentration for phosphorus uptake (g P m^{-2})
7	KHRB	Real	Dissolved oxygen concentration at which half of algal metabolism is released as dissolved organic carbon (g DO m^{-3})
1	BMRB	Real	Basal metabolic rate of algae at reference temperature (d^{-1})
2	BPRB	Real	Predation rate on algae at reference temperature (d^{-1})
3	KTBB	Real	Effect of temperature on metabolism and predation ($^oC^{-1}$)
4	TRB	Real	Reference temperature for specification of metabolism and predation (^{o}C)
5	BALGMIN	Real	Minimum allowable benthic algal biomass (g C m^{-2})
1	FNIB	Real	Fraction of inorganic nitrogen produced by metabolism and predation ($0 \leq FNIB \leq 1$)
2	FPIB	Real	Fraction of inorganic phosphorus produced by metabolism and predation ($0 \leq FPIB \leq 1$)

Example

```
BALGC
  OFF

   PMB     ANCB     APCB    KTGB1    KTGB2      TMB
 300.    0.167   0.0167    0.004    0.006     20.

ALPHB    CCHLB    KESED   KEBALG     KHNB     KHPB     KHRB
 4.25     75.0      0.5     0.01     0.01    0.001      0.5

 BMRB     BPRB     KTBB      TRB  BALGMIN
 0.01     0.01    0.069     20.     0.01
```

```
    FNIB     FPIB
     0.0      0.0
```

Net Settling Velocity

Net settling from the water column to sediments may be applied uniformly throughout the domain or may be varied spatially. The option to vary these spatially is useful if different depositional environments can be identified. This group of inputs consists of a header line, a line of character inputs, a blank line, another header line, a blank line and a list of settling velocities. This formatting is awkward but must be followed carefully. The first parameter list (//8X,2A8) specifies spatially-uniform or varying parameter assignment. For spatially-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to spatially-varying parameter assignment. Parameter values for all cells are echoed to the output file. The second parameter list specifies parameter values (:///(8X,7F8.1)). One line of parameter values is required for CONSTANT specification. Otherwise, one line must be entered for each sediment cell in the model grid. Sediment cell numbers correspond to water-column cell numbers in the surface layer. For convenience, the cell number may be entered in the first eight columns. This number is not read into the program. Parameters are understood to be in order starting from cell 1 up to the highest sediment cell number.

Field	Name	Value	Description
1	SPVARS	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTS	Character	Not activated
1	WSSNET	Real	Net settling velocity of inorganic solids to sediments (m d^{-1})
2	WSLNET	Real	Net settling velocity of labile particles to sediments (m d^{-1})
3	WSRNET	Real	Net settling velocity of refractory particles to sediments (m d^{-1})
4	WSCNET	Real	Net settling velocity of algal group 1 to sediments (m d^{-1})
5	WSDNET	Real	Net settling velocity of algal group 2 to sediments (m d^{-1})
6	WSGNET	Real	Net settling velocity of algal group 3 to sediments (m d^{-1})
7	WSUNET	Real	Net settling velocity of particulate biogenic silica to sediments (m d^{-1})

Example

```
      SPVARS  PRINTS
    CONSTANT      NO

  BOX  WSSNET  WSLNET  WSRNET  WSCNET  WSDNET  WSGNET  WSUNET

    1   0.500   0.500   0.500   0.000   0.500   0.100   0.010
```

Burial and Mixing Parameters

Burial to the inactive deep sediments, particle mixing, and porewater diffusion are input next. These may be applied uniformly across the system or varied spatially. This group of inputs consists of a header line, a line of character inputs, a blank line, another header line, a blank line and a list of settling velocities. This formatting is awkward but must be followed carefully. The first parameter list (//8X,2A8) specifies spatially-uniform or varying parameter assignment. For spatially-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to spatially-varying parameter assignment. Parameter values for all cells are echoed to the output file. The second parameter list specifies parameter values (:///(8X,7F8.1)). One line of parameter values is required for CONSTANT specification. Otherwise, one line must be entered for each sediment cell in the model grid. Sediment cell numbers correspond to water-column cell numbers in the surface layer. For convenience, the cell number may be entered in the first eight columns. This number is not read into the program. Parameters are understood to be in order starting from cell 1 up to the highest sediment cell number.

Field	Name	Value	Description
1	SPVARS	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTS	Character	Not activated
1	VSED	Real	Burial velocity to deep inactive sediments (cm yr^{-1})
2	VPMIX	Real	Particle mixing coefficient (m^2 d^{-1})
3	VDMIX	Real	Porewater diffusion coefficient (m^2 d^{-1})

Example

```
        SPVARS  PRINTS
      CONSTANT      NO

   BOX    VSED   VPMIX   VDMIX

     1   0.250 0.00012 0.00100
```

Coupling Water Column and Sediment Organic Matter

The water quality model has two classes of organic particulate matter: labile and refractory. The sediment model has three classes: G1 (labile), G2 (refractory), G3 (slow refractory or inert). The labile particles from the water column are routed to the G1 component of the sediment model. The water quality model refractory particles must be mapped into G2 and G3 particles in the sediment. This mapping usually corresponds to the fractionation specified for algae although particle splits may be spatially varied, if desired. The option to vary these is useful if particles that originate from a source other than phytoplankton (a river inflow or point-source discharge) are locally dominant.

This group of inputs consists of a header line, a line of character inputs, a blank line, another header line, a blank line and a list of settling velocities. This

formatting is awkward but must be followed carefully. The first parameter list (//8X,2A8) specifies spatially-uniform or varying parameter assignment. For spatially-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to spatially-varying parameter assignment. Parameter values for all cells are echoed to the output file. The second parameter list specifies parameter values (:///(8X,7F8.1)). One line of parameter values is required for CONSTANT specification. Otherwise, one line must be entered for each sediment cell in the model grid. Sediment cell numbers correspond to water-column cell numbers in the surface layer. For convenience, the cell number may be entered in the first eight columns. This number is not read into the program. Parameters are understood to be in order starting from cell 1 up to the highest sediment cell number.

Field	Name	Value	Description
1	SPVARS	Character	Spatially uniform (CONSTANT) or varying parameter specification
2	PRINTS	Character	Not activated
1	FRG2P	Real	Fraction water column refractory phosphorus routed into sediment model G2 class
2	FRG3P	Real	Fraction water column refractory phosphorus routed into sediment model G3 class
3	FRG2N	Real	Fraction water column refractory nitrogen routed into sediment model G2 class
4	FRG3N	Real	Fraction water column refractory nitrogen routed into sediment model G3 class
5	FRG2C	Real	Fraction water column refractory carbon routed into sediment model G2 class
6	FRG3C	Real	Fraction water column refractory carbon routed into sediment model G3 class

Example

```
          SPVARS  PRINTS
        CONSTANT      NO

    BOX   FRG2P   FRG3P   FRG2N   FRG3N   FRG2C   FRG3C

      1   0.255   0.095   0.300   0.050   0.300   0.050
```

Recapitulation

The inputs to the predictive sediment model are a mixture of formats including a number of blank and header lines. These can be difficult to visualize when broken into segments, as above. We present here a complete input deck showing proper formatting.

User-Specified Sediment-Water Fluxes

The Benthic Flux Input File has two formats. The appropriate format depends on the specification of SEDC and BFC in the Control File. If SEDC = "ON" the file contains input to the predictive sediment submodel. If BFC = "ON" the file contains user-specified specified benthic fluxes. If both parameters are "OFF" the file is not opened. This chapter describes input of user-specified sediment-water fluxes.

The first three lines of the file are reserved for comments and identification. Three card groups, each consisting of a header and input, follow. These groups specify parameters in the functions that relate specified fluxes to temperature and other influences (refer to the chapter on "Sediment-Water Interactions"). The remainder of the file is occupied by specified fluxes. Fluxes must be specified once at commencement of the model run. Fluxes may be updated at arbitrary intervals throughout the run.

Temperature Effects Card

Field	Name	Value	Description
1	KSDOC	Real	Effect of temperature on dissolved organic carbon flux
2	KSNH4	Real	Effect of temperature on ammonium flux
3	KSNO3	Real	Effect of temperature on nitrate flux
4	KSPO4	Real	Effect of temperature on phosphate flux
5	KSO	Real	Effect of temperature on sediment oxygen demand
6	KSSA	Real	Effect of temperature on silica flux

EXAMPLE

```
  KSDOC   KSNH4   KSNO3   KSPO4     KSO    KSSA
0.0693  0.0693  0.0693  0.0693  0.0693  0.0693
```

FORMAT

(8X,9F8.0)

Temperature Effects

Field	Name	Value	Description
1	TRSDOC	Real	Reference temperature for dissolved organic carbon flux
2	TRSNH4	Real	Reference temperature for ammonium flux
3	TRSNO3	Real	Reference temperature for nitrate flux
4	TRSPO4	Real	Reference temperature for phosphate flux
5	TRSOD	Real	Reference temperature for sediment oxygen demand
6	TRSSA	Real	Reference temperature for silica flux

EXAMPLE

```
TRSDOC  TRSNH4  TRSNO3  TRSPO4   TRSOD   TRSSA
  20.0    20.0    20.0    20.0    20.0    20.0
```

FORMAT

(://8X,9F8.0)

Additional Parameters

Field	Name	Value	Description
1	MTCNO3	Real	Nitrate mass transfer coefficient (m day^{-1})
2	SEDNO3	Real	Interstitial nitrate concentration (gm m^{-3})
3	KHSO	Real	Dissolved oxygen at which sediment oxygen consumption is halved (gm m^{-3})

EXAMPLE

```
MTCNO3  SEDNO3    KHSO
   0.1    0.00    2.00
```

FORMAT

(://8X,9F8.0)

Benthic Fluxes

Field	Name	Value	Description
1	Jday	Real	Julian day
2-9	Flux	Real	Benthic flux (gm m^{-2} day^{-1})

EXAMPLE

```
DOC           0.0  1.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000 0.0000
                   0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000 0.0000
```

FORMAT

(8X,9F8.0,:/(:16X,8F8.0))

Example of User-Specified Benthic Flux File

In the following example, fluxes are specified at Julian day 0 and revalued at day 110.

```
BENTHIC FLUX FILE FOR THIRTY-BOX BAY MODEL
FEBRUARY 22, 1994

           KSDOC   KSNH4   KSNO3   KSPO4     KSO    KSSA
          0.0693  0.0693  0.0693  0.0693  0.0693  0.0693

          TRSDOC  TRSNH4  TRSNO3  TRSPO4   TRSOD   TRSSA
            20.0    20.0    20.0    20.0    20.0    20.0

          MTCNO3  SEDNO3    KHSO
             0.1    0.00    2.00

    PARM    JDAY G/M2/DY G/M2/DY G/M2/DY G/M2/DY G/M2/DY G/M2/DY G/M2/DY G/M2/DY
DOC          0.0  1.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
NH4          0.0  0.1000  0.0100  0.0700  0.0700  0.0700  0.0700  0.0700  0.0700
                  0.0700  0.0700
NO3          0.0  0.1000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
DON          0.0  1.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
PO4          0.0  0.1000  0.0100  0.0090  0.0090  0.0090  0.0090  0.0090  0.0090
                  0.0090  0.0090
DOP          0.0  1.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
COD          0.0  1.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
SOD          0.0 -1.4500 -1.4500 -1.4500 -1.4500 -1.4500 -1.4500 -1.4500 -1.4500
                 -1.4500 -1.4500
DSIL         0.0  1.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
DOC        110.0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
NH4        110.0  0.0700  0.0700  0.0700  0.0700  0.0700  0.0700  0.0700  0.0700
                  0.0700  0.0700
NO3        110.0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
DON        110.0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
PO4        110.0  0.0090  0.0090  0.0090  0.0090  0.0090  0.0090  0.0090  0.0090
                  0.0090  0.0090
DOP        110.0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
COD        110.0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
SOD        110.0 -1.4500 -1.4500 -1.4500 -1.4500 -1.4500 -1.4500 -1.4500 -1.4500
                 -1.4500 -1.4500
DSIL       110.0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
                  0.0000  0.0000
```

The Suspension Feeder Input File

The Suspension Feeder Input File provides input to the suspension-feeder portion of the benthos model. The file has three parts. First, header information and a few miscellaneous parameters are specified. Next, parameters for each of the suspension-feeding species are input. Finally, the spatial distribution of the species is provided.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe suspension feeder input deck

Two title lines are required to describe the suspension feeder input deck. These are not read as variables but are skipped by a FORMAT statement.

Example

```
First run with new benthos model. NEW 12985 CELL grid
Identical to Run 47.  Feb. 10, 2000
```

Miscellaneous Parameters

Following a title line, the number of suspension feeder species (://(2I10)) and the distribution of algal silica (//F10.1) are specified. Each input consists of a blank line, a header line, and a data line. The number of species must be less than or equal NSFFP specified in the PARAMETER statement in file wqm_com.inc.

Field	Name	Value	Description
1	NSPECS	Integer	Number of suspension feeder species
1	FRSASF	Real	Fraction of algal silica recycled in dissolved form as a result of grazing ($0 \leq$ FRSASF ≤ 1)

Species-Specific Parameters

Parameter inputs for each species are grouped in five lines: a header line, three lines of data, and a blank line. The header is not read as a variable but is skipped by a FORMAT statement. The format for the data inputs is (8F10.3)

Field	Name	Value	Description
1	FILT	Real	Base filtration rate (L mg^{-1} C d^{-1})
2	SFA1	Real	Assimilation efficiency for algal group 1 ($0 \leq SFA1 \leq 1$)
3	SFA2	Real	Assimilation efficiency for algal group 2 ($0 \leq SFA2 \leq 1$)
4	SFA3	Real	Assimilation efficiency for algal group 3 ($0 \leq SFA3 \leq 1$)
5	SFA4	Real	Assimilation efficiency for labile particulate organic matter ($0 \leq SFA4 \leq 1$)
6	SFA5	Real	Assimilation efficiency for refractory particulate organic matter ($0 \leq SFA5 \leq 1$)
7	MAXING	Real	Maximum ingestion rate (mg prey C mg^{-1} C d^{-1})
8	SFCN	Real	Carbon-to-nitrogen ratio (mg C mg^{-1} N)
1	SFCP	Real	Carbon-to-phosphorus ratio (mg C mg^{-1} N)
2	SFRESP	Real	respiration rate at 20 ^oC (d^{-1})
3	SFPRED	Real	predation rate at 20 ^oC (m^2 mg^{-1} filter feeder C d^{-1})
4	SFTMN	Real	Minimum temperature for functioning of filter feeders (^oC)
5	THTAFILT	Real	Constant that controls temperature dependence of filtration
6	THTARESP	Real	Constant that controls temperature dependence of respiration
7	THTAPRED	Real	Constant that controls temperature dependence of predation
1	XKPO2	Real	Dissolved oxygen concentration at which predation on filter feeders is halved (g DO m^{-3})
2	SFTD	Real	time to death for 99% of the population (d)
3	FILTFACT	Real	exponent that relates filtration rate to areal biomass density
4	RESPFACT	Real	exponent that relates respiration rate to areal biomass density
5	SFDOH	Real	Dissolved oxygen concentration at which value of logistic function is one-half (g DO m^{-3})

6	SFDOQ	Real	Dissolved oxygen concentration at which value of logistic function is one-quarter (g DO m^{-3})
7	SFATURB	Real	Parameter that relates percent reduction to solids concentration
8	SFBTURB	Real	Parameter that relates percent reduction to solids concentration

Example

```
SPECIES 1 = Rangia cuneata  FILT 25%
     0.109     0.800     0.800     0.800     0.800       0.0      0.24      5.67
    45.000     0.026    0.5e-6     1.000     1.080     1.080     1.120
     1.000    14.000     0.422     0.119     1.000       0.7      81.0      24.0
```

Spatial Distribution of Suspension Feeders

The final portion of the input deck consists of a single header line and one data line for each cell in the surface plane of the model grid. (Suspension feeders are located in sediment cells that are numbered identically to the surface cell in the overlying water column.) Parameters are read in starting with Cell 1 and increasing to the highest cell number (I6,10(I4,F10.1)). Cell number may be inserted at the beginning of each line, but this number is not used by the program. Two columns are required for each suspension feeder species. The first column contains a binomial variable that indicates if the species is active in the cell. (0=inactive, 1=active.) The second number is the initial biomass in the cell. As presently coded, this biomass is overwritten when initial conditions are subsequently input.

Field	Name	Value	Description
1	BOX	Integer	Cell number
2	SEDTYPE	Integer	Sepcies is active (=1) or inactive (=0)
3	BIOMASS	Real	Initial biomass (mg C m^{-2})

Example

```
   BOX SED   BIOMASS SED   BIOMASS SED   BIOMASS SED   BIOMASS
     1   1    3000.0   1    3000.0   0      10.0
     2   1    3000.0   1    3000.0   0      10.0
     3   0      10.0   1    3000.0   0      10.0
     4   1    3000.0   1    3000.0   0      10.0
     5   0      10.0   1    3000.0   0      10.0
     6   1    3000.0   1    3000.0   0      10.0
     .   .        .    .        .    .        .
     .   .        .    .        .    .        .
     .   .        .    .        .    .        .
  2956   0      10.0   0      10.0   0      10.0
  2957   0      10.0   0      10.0   0      10.0
  2958   0      10.0   0      10.0   0      10.0
  2959   0      10.0   0      10.0   0      10.0
  2960   0      10.0   0      10.0   0      10.0
  2961   0      10.0   0      10.0   0      10.0
```

Recapitulation

The inputs to the suspension feeder model are a mixture of formats including a number of blank and header lines. These can be difficult to visualize when broken into segments, as above. We present here a complete input deck showing proper formatting.

```
First run with new benthos model. NEW 12985 CELL grid
Identical to Run 47.  Feb. 10, 2000

    NSPECS         # of species
         3

    FRSASF      Fraction of avail Si (SA) recycled from diatom grazing
     0.300

 SPECIES 1 = Rangia cuneata  FILT 25%
     0.109     0.800     0.800     0.800     0.800       0.0      0.24      5.67
    45.000     0.026    0.5e-6     1.000     1.080     1.080     1.120
     1.000    14.000     0.422     0.119     1.000       0.7      81.0      24.0

 SPECIES 2 = Macoma balthica  FILT 25%
     0.163     0.800     0.800     0.800     0.800     0.000     0.240     5.670
    45.000     0.026    1.0e-6     1.000     1.080     1.080     1.120
     1.000    14.000     0.431     0.119     1.000     0.700      81.0      24.0

 SPECIES 3 = Corbicula fluminea  FILT 50%
     0.216     0.800     0.800     0.800     0.800     0.000     0.240     5.670
    45.000     0.026    0.2e-6     1.000     1.080     1.080     1.120
     1.000    14.000     0.422     0.119     1.000     0.700      81.0      24.0

   BOX SED   BIOMASS SED   BIOMASS SED   BIOMASS SED   BIOMASS
     1   1    3000.0   1    3000.0   0      10.0
     2   1    3000.0   1    3000.0   0      10.0
     3   0      10.0   1    3000.0   0      10.0
     4   1    3000.0   1    3000.0   0      10.0
     5   0      10.0   1    3000.0   0      10.0
     6   1    3000.0   1    3000.0   0      10.0
     .   .        .    .        .    .        .
     .   .        .    .        .    .        .
     .   .        .    .        .    .        .
  2956   0      10.0   0      10.0   0      10.0
  2957   0      10.0   0      10.0   0      10.0
  2958   0      10.0   0      10.0   0      10.0
  2959   0      10.0   0      10.0   0      10.0
  2960   0      10.0   0      10.0   0      10.0
  2961   0      10.0   0      10.0   0      10.0
```

Submerged Aquatic Vegetation Model

Introduction

Submerged aquatic vegetation (SAV) was introduced to CE-QUAL-ICM during the tributary refinements phase of the Chesapeake Bay study (Cerco and Moore 2001, Cerco et al. 2002). Subsequently, the model was modified for application to Florida Bay (Cerco et al. 2000). The Chesapeake Bay version of the model is included in the Lake Washington code. Two major differences distinguish the Chesapeake Bay and Florida Bay applications. In Chesapeake Bay, multiple SAV species are mutually exclusive; in Florida Bay, multiple species compete. Epiphytes attached to SAV are dynamically computed in Chesapeake Bay. Epiphytes take a specified, constant value in Florida Bay.

Three components are required to make up a system-wide SAV model. The first is a unit-level model of a plant. The second is an environmental model that provides light, temperature, nutrient concentrations, and other forcing functions to the plant component. The third is a coupling algorithm that links the system-wide environmental model to the local-scale plant model. The unit model and the coupling algorithm are described below.

The Submerged Aquatic Vegetation Unit Model

The SAV unit model (Fig. 1) incorporates three state variables: shoots (above-ground biomass), roots (below-ground biomass), and epiphytes (attached growth). Epiphytes and shoots exchange nutrients with the water-column component of the eutrophication model while roots exchange nutrients with the diagenetic sediment component (see "Sediment-Water Interactions" chapter). Light available to the shoots and epiphytes is computed via a series of sequential attenuations by color, fixed and organic solids in the water column, and by self-shading of shoots and epiphytes. The selection of state variables and basic principles of the model are based on principles established by Wetzel and Neckles (1986) and Madden and Kemp (1996).

Shoots

The governing equation for shoots establishes a balance between sources and sinks of above-ground biomass:

$$\frac{d\,SH}{dt} = (P \cdot (1 - Fpsr) - Rsh - SL) \cdot SH + Trs \cdot RT \qquad \textbf{(1)}$$

in which SH = shoot biomass (g C m^{-2}); P = production (d^{-1}); Fpsr = fraction of production routed from shoot to root; Rsh = shoot respiration (d^{-1}); SL = sloughing (d^{-1}); Trs = rate at which carbon is transported from root to shoot (d^{-1}); and RT = root biomass (g C m^{-2}).

Production is computed as the product of a specified maximum rate (a function of temperature) and a limiting factor. The limiting factor is the minimum of independently evaluated light, nitrogen, and phosphorus limitations. Light limitation is selected from one of several functions (Jassby and Platt 1976) that fit observed production versus irradiance curves:

$$f(I) = \frac{Ish}{\sqrt{Ish^2 + Ik^2}} \qquad \textbf{(2)}$$

in which f(I) = light limitation; and Ish = irradiance at leaf surface (E m^{-2} day^{-1}). Parameter Ik is derived from two specified parameters:

$$Ik = \frac{\mathrm{Pmax}(T)}{\alpha} \qquad \textbf{(3)}$$

in which Pmax = maximum production as a function of temperature (g C g^{-1} DW d^{-1}) and α = initial slope of production versus irradiance curve (g C g^{-1} DW) (E m^{-2})$^{-1}$.

Nutrient limitations for nitrogen and phosphorus are evaluated using a formula (Madden and Kemp 1996) that combines individual Monod-like functions for the roots and shoots:

$$f(N) = \frac{Nw + K^* \cdot Ns}{Khw + Nw + K^* \cdot Ns} \qquad \textbf{(4)}$$

in which f(N) = nutrient limitation; Nw = nutrient concentration (g m^{-3}) in water column, Ns = nutrient concentration (g m^{-3}) in sediment pore water; Khw = half-saturation concentration for nutrient uptake by shoots (g m^{-3}); Khs = half-saturation concentration for nutrient uptake by roots (g m^{-3}); and K^* = Khw / Khs.

Roots

The governing equation for roots establishes a balance between sources and sinks of below-ground biomass:

$$\frac{d\,RT}{dt} = Fpsr \cdot P \cdot Sh - Rrt \cdot RT - Trs \cdot RT \qquad \textbf{(5)}$$

in which Rrt = root respiration (d^{-1}).

Epiphytes

Epiphytes are quantified as mass per unit of shoot mass:

$$\frac{d\,EP \cdot SH}{dt} = (Pep \cdot DL - BMep - PR \cdot EP - SL) \cdot SH \cdot EP \qquad \textbf{(6)}$$

in which EP = epiphyte abundance (g epiphyte C g^{-1} shoot carbon); Pep = epiphyte production (d^{-1}); DL = density limitation function; BMep = epiphyte respiration (d^{-1}); and PR = predation on epiphytes (g shoot C g^{-1} epiphyte carbon d^{-1}).

The formulation provides a change in epiphyte abundance as a function of epiphyte processes and shoot processes. Net production of epiphytes without corresponding production of shoots results in an increase in epiphyte abundance on the shoots. Net production of shoots without corresponding epiphyte production results in diminished epiphyte abundance. Sloughing results in loss of attached epiphytes and produces no net change in abundance. The density limitation function diminishes production as leaf substrate becomes filled with epiphytes.

Epiphyte production is modeled as a function of light, nutrients, and temperature. Light effects are computed using formulae similar to Equations 2 and 3 while nutrient effects are evaluated with conventional Monod functions. Neckles et al. (1993) showed that predation can be an important limitation on epiphyte abundance. Absence of data prevents inclusion of predators in the model, however. Instead, a linear proportionality between predators and prey is assumed. Parameter PR incorporates both the proportionality and predation rate and is evaluated empirically.

SAV Composition and Nutrient Cycling

A fundamental assumption of the model is that plants have uniform, constant composition. Nitrogen and phosphorus in plant biomass are quantified as fractions of the carbonaceous biomass. Nutrients are taken up in stoichiometric relation to net production. Proportions removed from the water column and sediments are determined by the relative nutrient limits in each pool. Respiration and sloughing return appropriate quantities of nutrients to the sediments and water column.

The Light Field

A conceptual model has been long-established in which light reaching SAV shoots is first attenuated by dissolved and particulate matter in the water

column and next by epiphytic material (e.g. Kemp et al. 1983). The representation of self-shading by shoots and by epiphytes and potential shading of epiphytes by SAV is murkier. One approach is to incorporate density-limiting functions into the model that simulate both self-shading and space limitations (Wetzel and Neckles 1986; Madden and Kemp 1996). The density-limit approach is adopted here for epiphytes since it appears reasonable that epiphyte abundance will ultimately be limited by leaf substrate available for attachment. The concept of a space limitation on SAV shoots is less appealing, however. Consequently, self shading by SAV shoots is considered explicitly.

Light available to SAV shoots is computed through a series of sequential attenuations. First, light at the top of the canopy is computed:

$$Ic = Io \cdot e^{-(Kw + Ki \cdot Iss + Kv \cdot VSS) \cdot Ztc} \quad \textbf{(7)}$$

in which Ic = light at the canopy top (E m^{-2} day^{-1}); Io = light at water surface (E m^{-2} day^{-1}); Kw = attenuation due to color (m^{-1}); Ki = attenuation coefficient for fixed solids (m^2 g^{-1}); ISS = fixed solids concentration (g m^{-3}); Kv = attenuation coefficient for volatile solids (m^2 g^{-1}); VSS = volatile solids concentration (g m^{-3}); and Ztc = depth to canopy (m).

Next, mean light within the canopy is evaluated. Assuming that attenuation by shoots follows an exponential relationship analogous to Equation 7 (Titus and Adams 1979), the mean light field within the canopy is:

$$Iwc = \frac{Ic}{Ksh \cdot SH} \cdot (1 - e^{-Ksh \cdot SH}) \quad \textbf{(8)}$$

in which Iwc = mean light within the canopy (E m^{-2} day^{-1}); and Ksh = attenuation by SAV shoots (m^2 g^{-1} C). Iwc is the light available to epiphytes.

Although epiphyte accumulation in Chesapeake Bay and elsewhere can be related to nutrient concentrations (Kemp et al. 1983; Twilley et al. 1985; Borum 1985), not all epiphytic material is viable algae. Total accumulation of epiphytic material is an order of magnitude greater than viable algae (Fig. 2). A rough proportionality between total accumulation and biomass is maintained over several orders of magnitude of biomass. The proportionality is represented in the model by the quantity Adwcep, the ratio of total epiphyte dry weight to viable epiphyte carbon. Employing this parameter, light reaching the shoots through the epiphyte layer is computed:

$$Ish = Iwc \cdot e^{-Kep \cdot Acla \cdot Adwcep \cdot EP} \quad \textbf{(9)}$$

in which Ish = light available to shoots (E m^{-2} day^{-1}); Kep = attenuation by epiphytes (m^2 leaf surface g^{-1} DW); and Acla = g shoot C m^{-2} leaf area.

SAV Effect on Suspended Solids

The damping of wind-generated waves in SAV beds (Ward et al. 1984) results in diminished suspended sediment concentrations relative to

concentrations outside the bed (Fig. 3). The effect of SAV on suspended solids is represented by addition of an SAV-dependent net-settling velocity to the mass balance equation for suspended solids:

$$\frac{\delta Iss}{\delta t} = \text{Net transport} - \frac{1}{H} \cdot (Wiss + Wsav \cdot SH) \cdot ISS \qquad \textbf{(10)}$$

in which Wiss = net settling velocity of suspended solids in open water (m d^{-1}); Wsav = enhanced net settling due to SAV (m^3 g^{-1} C d^{-1}); and H = local depth (m). Parameter Wiss varies spatially and temporally but has a characteristic value 0.05 m d^{-1}. Value of Wsav, 0.05 m^3 g^{-1} C d^{-1}, is assigned to reproduce in the model the observed trend.

From the Unit to the System

The Chesapeake Bay Environmental Model Package (CBEMP) operates by dividing the continuum of the bay into a grid of discrete cells. In the Virginia Tributary Refinements, the surface plane of the bay and its major tributaries was sectioned into 2100 cells with a length scale of 2 km. Width of each cell varied depending on the local geometry. For the SAV model, a ribbon of littoral cells was created along the land-water margin of the system. Width of each littoral cell corresponded to the distance from the two-meter depth contour to the shore. The two-meter depth was selected since restoration of SAV to the two-meter contour was a major goal of the bay management effort. SAV was modeled in these littoral cells and in a few additional cells in regions that historically supported SAV. Littoral cells were represented as having a mean depth of one meter. Depth of the additional cells was determined by local bathymetry and was usually 2 m.

The major problem in coupling the system-wide model with the unit model is the difference in scales represented by the two models. The minimum scale represented by the CBEMP is on the order of km while the scale on which SAV is distributed is orders of magnitude smaller. Three scaling factors were employed to relate biomass on the unit level to abundance on the grid scale. These were: truncation error, coverage, and patchiness (Fig. 4). Truncation error is the ratio of actual area within the two-meter contour to the area of the quadrilateral model cell. Coverage is the fraction of a cell occupied by SAV beds, and patchiness represents the fraction of bottom area covered by plants within an SAV bed. Abundance within each cell is then:

$$M = SH \cdot A \cdot TE \cdot C \cdot P \qquad \textbf{(11)}$$

in which M = above-ground abundance (g C); A = cell surface area (m^2); TE = truncation error; C = coverage; and P = patchiness.

The relationship of shoot (and root) biomass to abundance allows uptake and release of materials by plants on a unit area basis to be converted to a mass basis for employment in the mass-balance equation applied to each cell (see "Kinetics" chapter). Coverage and patchiness are model input variables, required for mass balance purposes. Truncation error is used in a model postprocessor to

relate observed and computed abundance.

Model Communities

Primary data base for comparison of computed and observed SAV was a monthly time series of above-ground abundance estimates (Moore et al. 2000) for the period 1985-1996. Estimates were provided for four mutually-exclusive SAV community types and were available on an aggregate basis and for each of 44 Chesapeake Bay Program Segments (CBPS). Program segments are subdivisions of the bay determined by mean salinity, natural boundaries, and other features. Thirty-five segments (Fig. 5), having a median area of 150 km^2, were included in the model grid.

Three major, mutually-exclusive SAV community types were modeled: ZOSTERA, RUPPIA, and FRESHWATER. Moore et al. (2000) identified a fourth type, POTAMOGETON, but the abundance in this type was negligible compared to the others. Since the distributions of POTAMOGETON and RUPPIA often overlap, the POTAMOGETON community was combined into the RUPPIA community for model purposes. Model cells were assigned a community type (Fig. 6) based on observed distribution and environmental factors.

Parameter Evaluation

Parameters for the SAV model were developed at the time of initial model application (Cerco et al. 2002). When phytoplankton production relationships and parameters in the eutrophication model were subsequently revised, corresponding changes were made to the epiphyte component of the SAV model. One potentially significant alteration was a change from daily-average irradiance to sinusoidally-varying irradiance. Examination of the SAV component of the model revealed that these changes had a substantial effect on computed SAV. As a consequence, a re-calibration of the SAV model was completed. We endeavored to bring epiphytes and SAV back into calibration while minimizing revisions to the original model parameter suite. Changes were centered on the epiphyte loss terms and on the SAV production-irradiance relationships. Parameter values reported here are from the most recent Chesapeake Bay application (Cerco and Noel 2004).

The SAV Component

Parameter evaluation for the SAV component of the model is both an art and a chore. Although substantial observations exist, especially for the ZOSTERA community, variations in methodology and reporting preclude determination of a definitive set of model parameters. The evaluation procedure consisted of selection of an initial parameter set from the literature, followed by revisions to improve agreement between modeled and observed biomass in CBPS that support substantial SAV communities.

For ZOSTERA, primary data sources included Wetzel and Penhale (1983), Evans et al. (1986), and Marsh et al. (1986). Parameters (Table 1) were

selected to optimize agreement between computed and observed shoot and root biomass (Fig. 7). For RUPPIA, primary data sources were Wetzel and Penhale (1983) and Evans et al. (1986). Final parameters (Table 1) were selected to optimize agreement between computed and observed shoot (Fig. 8) and root biomass. Insufficient data were found to assemble monthly means and ranges of root biomass. Observations collected by Moore et al. (1994) over a year indicated a range in root biomass of 0.8 to 13 g C m^{-2} with a mean of 6.1 g C m^{-2}. For the FRESHWATER community, primary data sources included Van et al. (1976), Bowes et al (1977; 1979), and Barko and Smart (1981). Final parameters (Table 1) were selected to optimize agreement between computed and observed shoot (Fig. 9) and root biomass. As with RUPPIA, insufficient data were found to assemble meaningful monthly means and ranges of root biomass. Available information indicated the roots of freshwater SAV comprise from 4% to 41% of total plant biomass (Haller and Sutton 1975, Barko and Smart 1981).

Epiphytes

Epiphyte accumulation on natural and artificial substrates has been measured at various locations in situ (Carter et al. 1985) and in artificial environments adjacent to the bay (Staver 1984, Twilley et al, 1985). For comparison with the model, reports of in-situ accumulation on natural substrates were desirable. The best data sets identified were collected from *Zostera marina* in the lower eastern shore of the bay (Moore et al. 1994), and in Bogue Sound (Penhale 1977), a lagoon situated 300 km south of the bay. Initial parameters for epiphytes were adapted from the phytoplankton component of the CBEMP. Final parameters (Table 2) were selected to obtain reasonable agreement between computed and observed epiphyte abundance (Fig. 10).

From the Unit to the System

Truncation error was determined by comparison of model surface area with actual area determined by a Geographical Information System. The error ranged from 0.2 to 1.55 with a mean value of 0.75. Coverage was assumed to be fifty percent. Patchiness was determined by comparison of computed and observed abundance and was determined to be 0.3 for the FRESHWATER and ZOSTERA communities and 0.8 for the RUPPIA community.

Model Application

The CBEMP was applied to the ten-year period 1985-1994. The eutrophication model, including the SAV component, was initialized once and run continuously through the simulated period. Boundary conditions and loads were updated on a daily or monthly basis. Integration time step was 15 minutes. Output from the model was stored at ten-day increments.

Agreement with Living-Resource Parameters

Living resource criteria for the survival and propagation of SAV in Chesapeake Bay were identified by Batiuk et al. (1992). The investigators

determined maximum light attenuation for survival of SAV at the one-meter depth to be 2.0 m^{-1} for freshwater species and 1.5 m^{-1} for saltwater species. Model results were compared to these criteria by plotting median shoot biomass in each cell for each of ten growing seasons (April - October) against median computed light attenuation. Shoot densities computed by the model clearly conform to the observed criteria (Fig. 11). Although computed SAV occasionally survives for a season under conditions that marginally exceed the criteria, the vast majority of computed biomass occurs in cells that meet the criteria. Model regions that substantially exceed the criteria never support SAV.

Effect on Suspended Solids

The influence of SAV on suspended solids was determined by collecting suspended solids observations inside and outside SAV beds. The modeled influence was examined by performing analogous observations on the model. Computed solids in cells that supported SAV were compared to computed solids in adjacent cells outside the SAV zone. As with the observations, considerable scatter occurs in the ratio (Fig. 12). The relationship (Equation 10) employed to simulate SAV effects on solids clearly works as desired, however, and model results are in reasonable agreement with the trend exhibited by observations.

Spatial Distribution of SAV and Light Attenuation

SAV abundance is not uniformly distributed in the bay system (Fig. 13). Within the mainstem bay and its major embayments, SAV is concentrated in CB1, near the confluence with the Susquehanna River, and in the lower half of the bay. Of the tributaries, only the tidal fresh and transitional portions of the Potomac River exhibit substantial abundance although lesser accumulations exist in the lower Rappahannock and York Rivers.

The observed distribution of SAV largely reflects the distribution of light attenuation (Fig. 14). The mainstem bay exhibits a classic turbidity maximum that typically occurs in CB2. Lesser attenuation occurs above and downstream of the maximum. Substantial SAV abundance is restricted to these same areas above and downstream of the maximum. The major tributaries are more turbid than most of the bay and, with the exception of portions of the Potomac, do not support substantial accumulations of SAV.

Trends in SAV

Moore et al. (2000) noted a substantial increase in ZOSTERA abundance from the period 1985 to 1990. Abundance of the other communities was less than ZOSTERA and exhibited no trend. Comparison of model results with time series of observed community abundance (Fig. 15) indicates the model represents correctly the relative abundance in each community. Inter-annual variability and trends are not well represented, however.

Discussion

The model performs well in computing the spatial distribution of SAV

(Fig. 13) but provides little information regarding inter-annual variability in abundance (Fig. 15). In the long term, the spatial distribution of SAV is determined by the area suited for SAV and by environmental factors, especially light attenuation. The areas are input to the model and the spatial distribution of environmental factors can be computed with reasonable accuracy. Consequently, the spatial distribution of SAV can be computed with corresponding accuracy.

Inter-annual variability in SAV abundance is affected by a host of factors. These include environmental influences that vary on numerous time scales and inherent properties of the biota. Short-term or localized events such as storm pulses can have a significant impact on SAV (Moore et al. 1997). Consistent, universal simulation of event-scale processes is currently beyond the capability of the CBEMP. Moreover, the response of the plants to events must also be represented. Consequently, improvements in computing year-to-year variability await both more accurate environmental models and improved representations of plant physiology.

A high priority for model improvement should be placed on models of plant propagation. This includes local propagation via roots and rhizomes and propagation over distances via seeds and plant fragments. The present model assumes a trace, refuge, population in each cell that is available for growth when conditions are favorable. In reality, change in the spatial extent of existing beds is limited by the rates of production and demise of plants at the edges of the beds. The appearance of SAV in new areas, depends on the transport of viable plant material or propagules to these areas. The ability to model year-to-year variation in abundance partially depends on the ability to model propagation as well as the ability to model the environment.

Lastly, the ability to model SAV on a sub-grid scale should be attained. One feasible approach is to divide the model cell into smaller SAV cells. Since bathymetry and other measures may not be available on the desired scale and since CBEMP computations are not available on the sub-grid scale, properties of the SAV cells could be distributed randomly with mean properties determined by the larger model. A second, more advanced approach would be to develop individual-based models of plants and propagate these within model cells.

Table 1
Parameters in SAV model

Parameter	Definition	Freshwater	Ruppia	Zostera	Units
Acdw	carbon to dry weight ratio	0.37	0.37	0.37	
Acla	shoot carbon per unit leaf area	7.5	4.0	4.0	g shoot C m^{-2} leaf area
Fpsr	fraction of production transferred from shoots to roots	0.12 to 1.0	0.1 to 0.85	0.1 to 0.85	
Ksh	light attenuation by shoots	0.045	0.045	0.045	m^2 g^{-1} C
Khnw	half-saturation concentration for nitrogen uptake by shoots	0.19	0.19	0.1	g N m^{-3}
Khns	half-saturation concentration for nitrogen uptake by roots	0.95	0.95	0.4	g N m^{-3}
Khpw	half-saturation concentration for phosphorus uptake by shoots	0.028	0.028	0.02	g P m^{-3}
Khps	half-saturation concentration for phosphorus uptake by roots	0.14	0.14	0.1	g P m^{-3}
Pmax	maximum production at optimum temperature	0.1	0.09	0.06	g C g^{-1} DW d^{-1}
Rsh	shoot respiration	0.02	0.015	0.013	d^{-1}
Rrt	root respiration	0.02	0.015	0.013	d^{-1}
SL	sloughing	0.01 to 0.1	0.01 to 0.035	0.01 to 0.035	d^{-1}
Trs	transfer from root to shoot	0.0 to 0.05	0.0	0.0	d^{-1}
α	initial slope of PvsI curve	0.015	0.0036	0.0068	(g C g^{-1} DW) (E m^{-2})$^{-1}$

Table 2
Parameters in epiphyte model

Parameter	Definition	Value	Units
Acchl	carbon to chlorophyll ratio of viable epiphytes	75	g C g^{-1} Chl
Adwcep	ratio of epiphyte dry weight to viable epiphyte carbon	18	g DW g^{-1} C
Kep	light attenuation coefficient	0.06	m^2 leaf surface g^{-1} epiphyte DW
Khep	density at which growth is halved	0.1	g epiphyte C g^{-1} shoot C
Khn	half-saturation concentration for nitrogen uptake	0.025	g N m^{-3}
Khp	half-saturation concentration for phosphorus uptake	0.0025	g P m^{-3}
Pep	maximum production at optimum temperature	350	g C g^{-1} Chl d^{-1}
PR	predation rate	5.0	g shoot C g^{-1} epiphyte C d^{-1}
BMep	respiration	0.025	d^{-1}
□	initial slope of PvsI curve	8	(g C g^{-1} Chl) (E m^{-2})$^{-1}$

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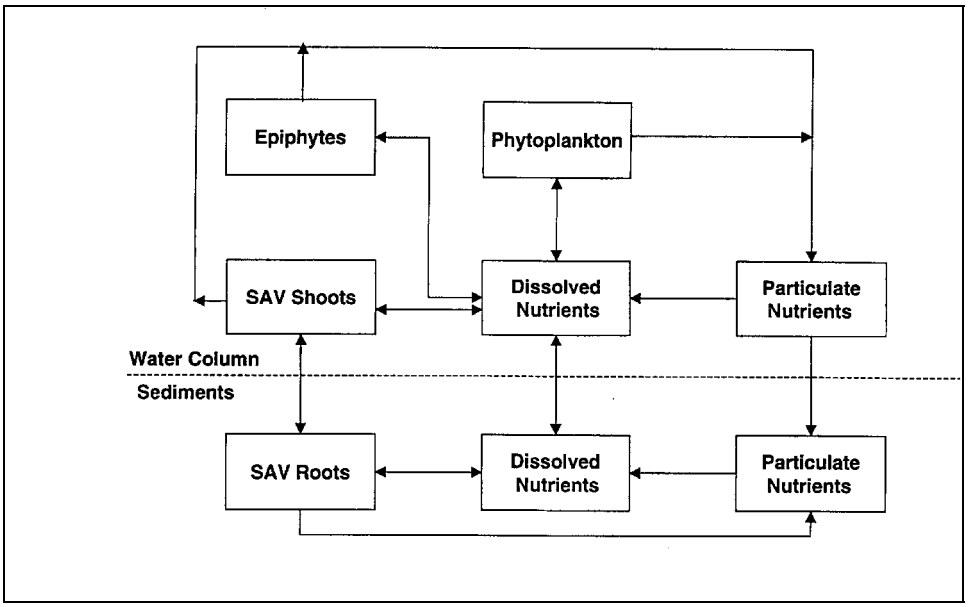


Figure 1. SAV model state variables (boxes) and mass flows (arrows).

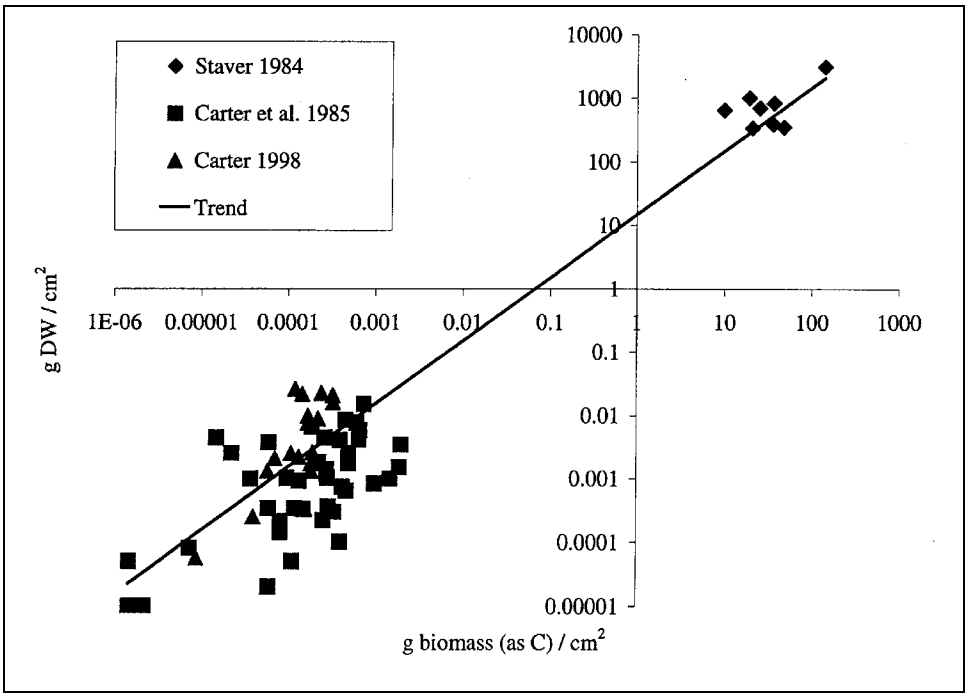


Figure 2. Epiphytic dry weight versus viable carbon. Staver's data from "control" and "low" ponds. Carbon obtained from chlorophyll measures using carbon-to-chlorophyll ratio of 75. Trend indicates a 15:1 ratio.

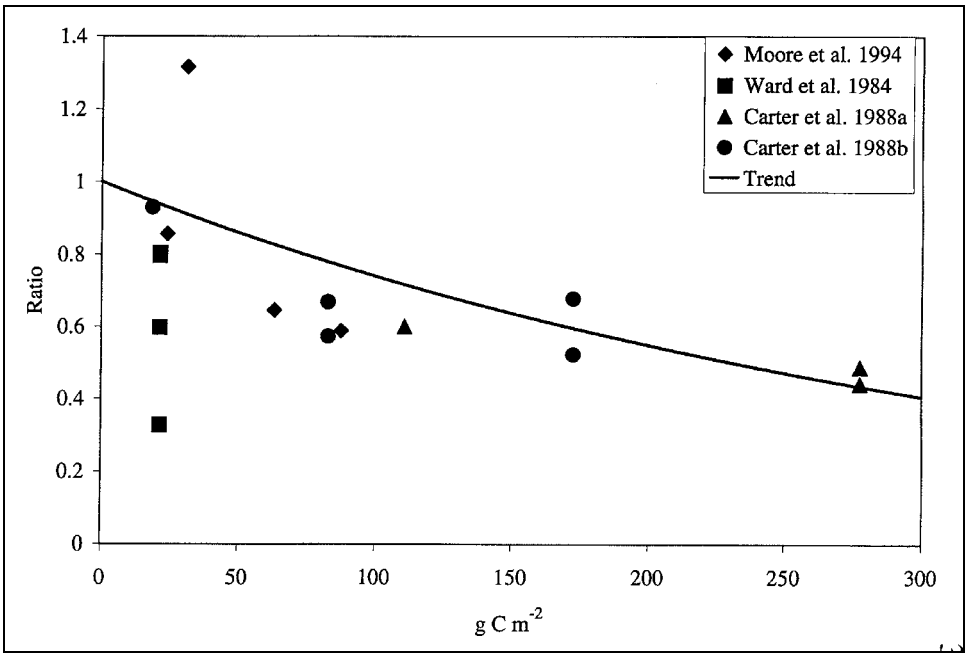


Figure 3. Ratio of suspended solids in vegetated areas to suspended solids in adjacent non-vegetated areas. Trend determined by visual comparison with observations.

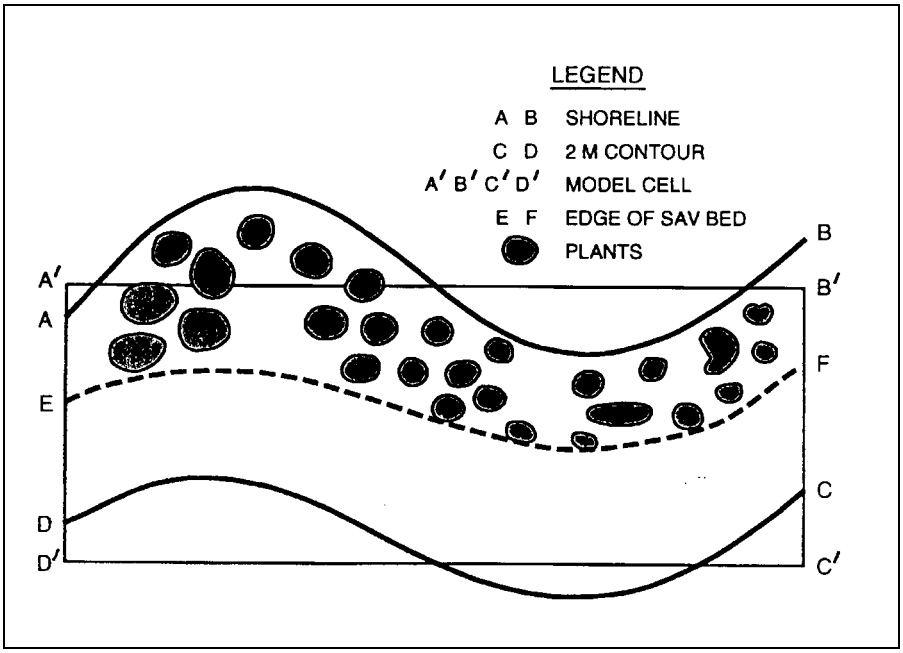


Figure 4. Truncation error, coverage, and patchiness. Truncation error = Area(ABCD)/Area(A'B'C'D'). Coverage = Area(ABEF)/Area(ABCD). Patchiness = Area(plants)/Area(ABEF).

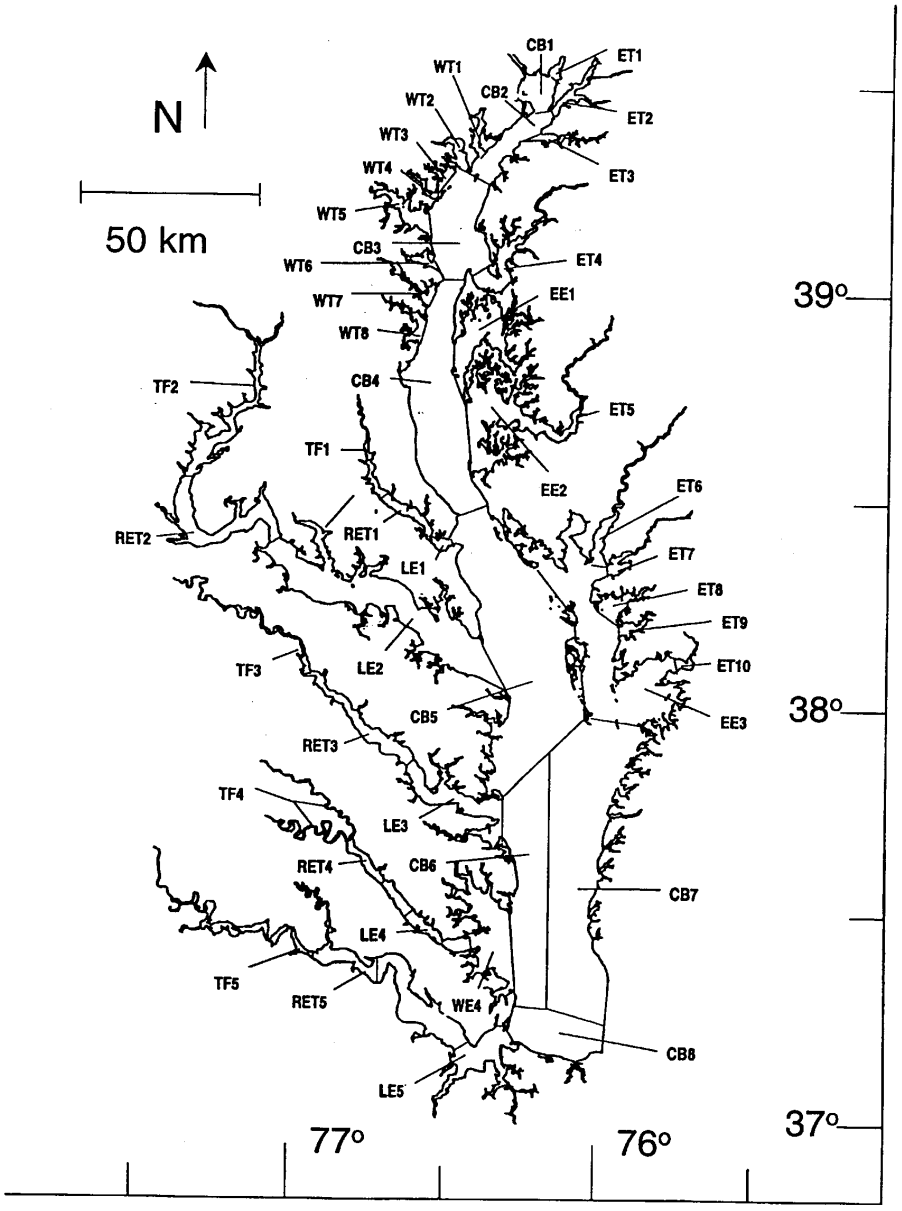


Figure 5. Chesapeake Bay Program Segments

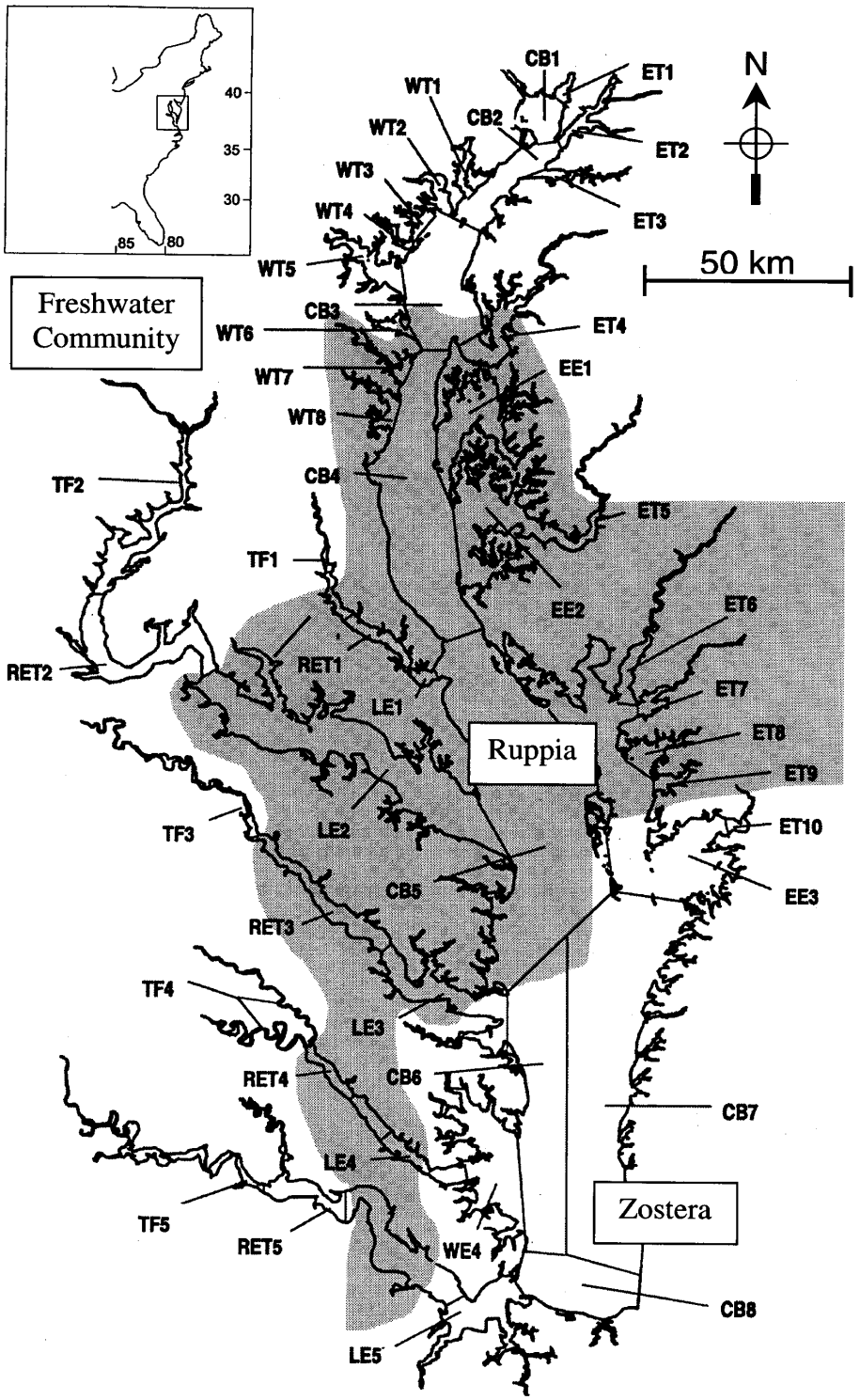


Figure 6. Distribution of SAV community types.

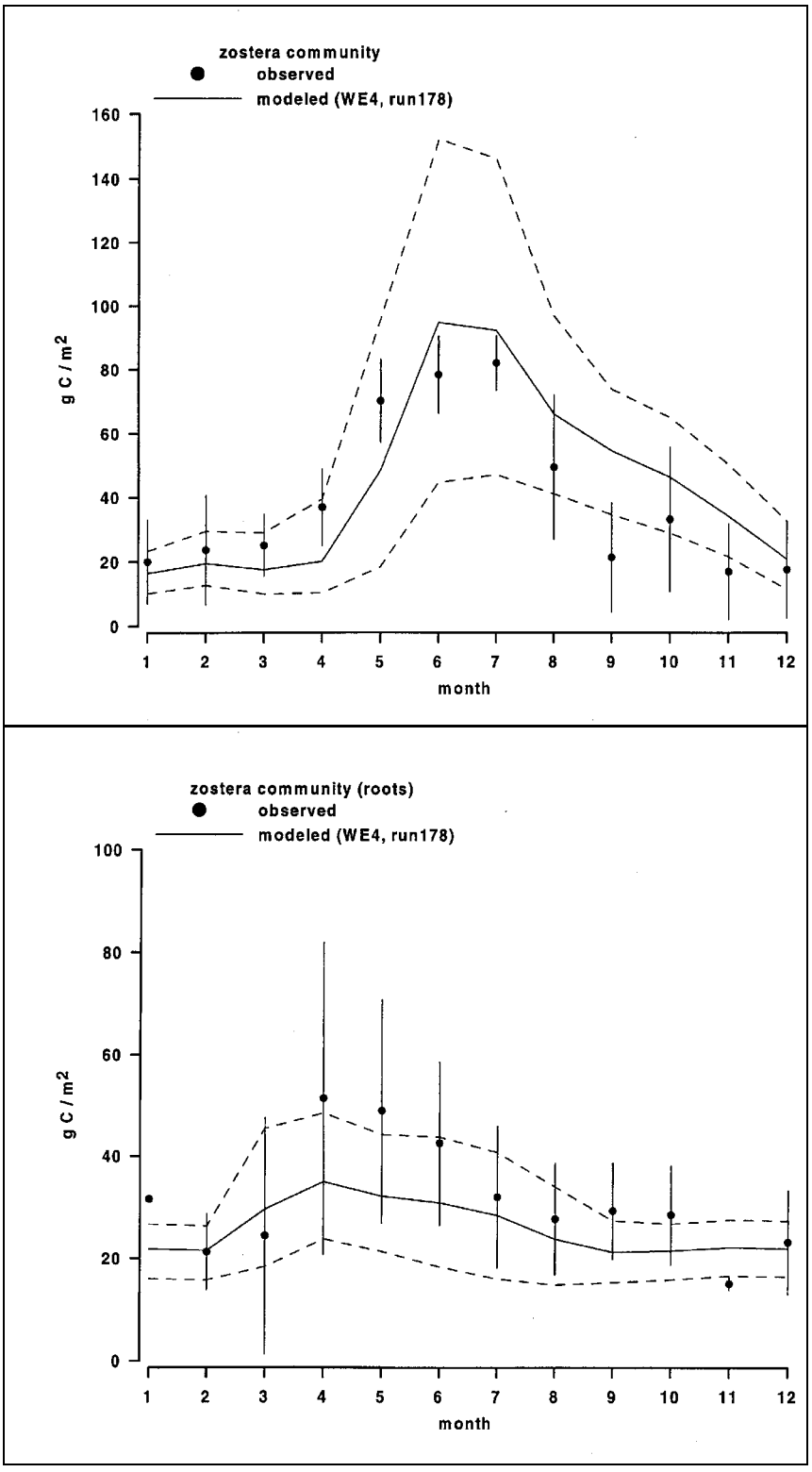


Figure 7. Modeled (mean and interval encompassing 95% of computations) and observed (mean and 95% confidence interval) ZOSTERA shoot (A) and root (B) biomass. Shoot observations from Moore et al. 1999. Root observations assembled from Moore et alia sources. Model results from CBPS WE4.

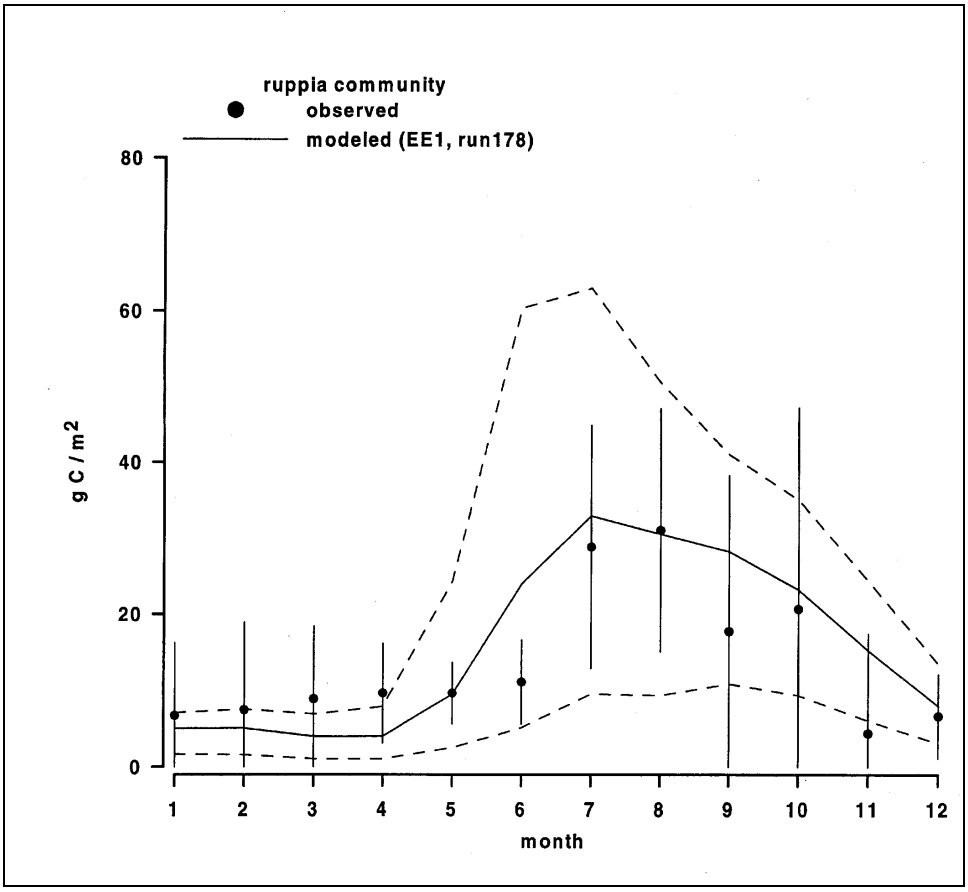


Figure 8. Modeled (mean and interval encompassing 95% of computations) and observed (mean and 95% confidence interval) RUPPIA shoot biomass. Observations from Moore et al. 1999. Model results from CBPS EE1.

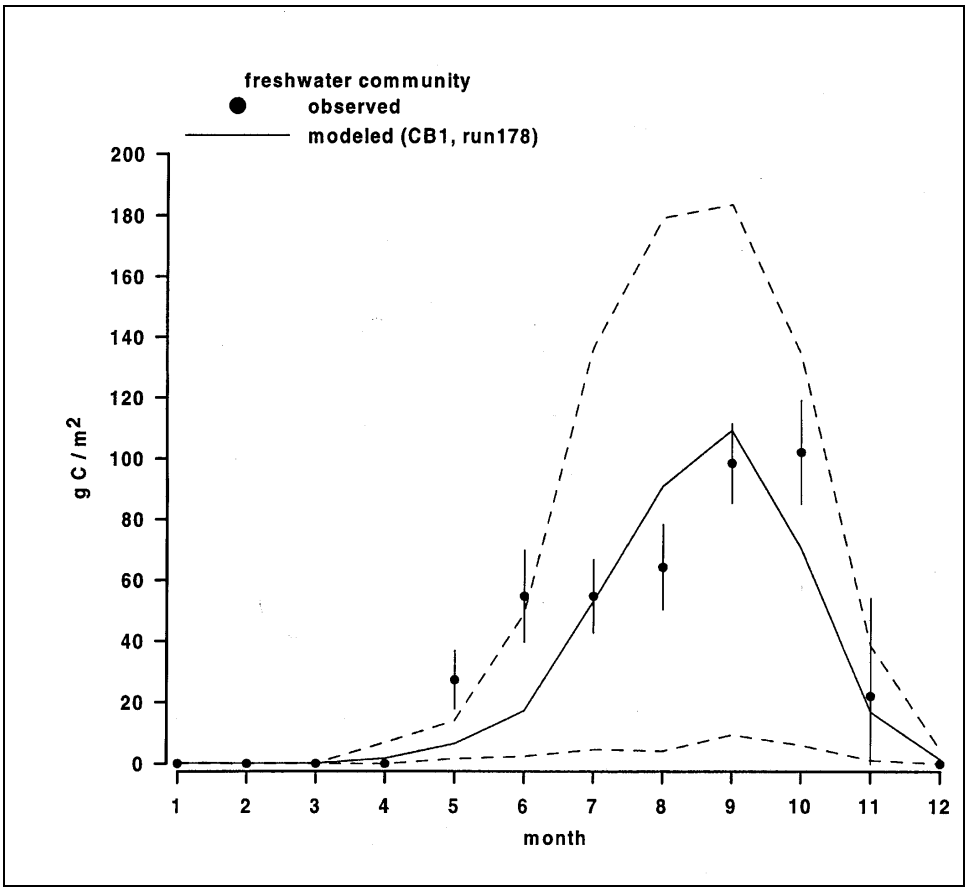


Figure 9. Modeled (mean and interval encompassing 95% of computations) and observed (mean and 95% confidence interval) FRESHWATER community shoot biomass. Observations from Moore et al. 1999. Model results from CBPS CB1.

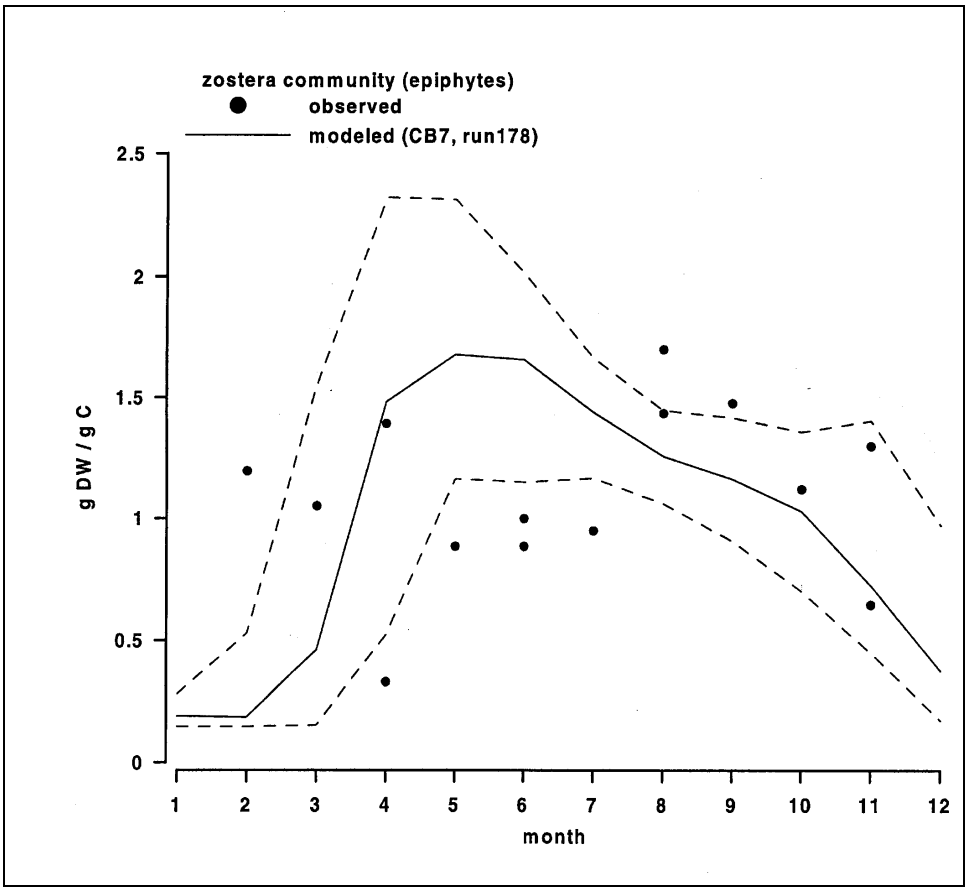
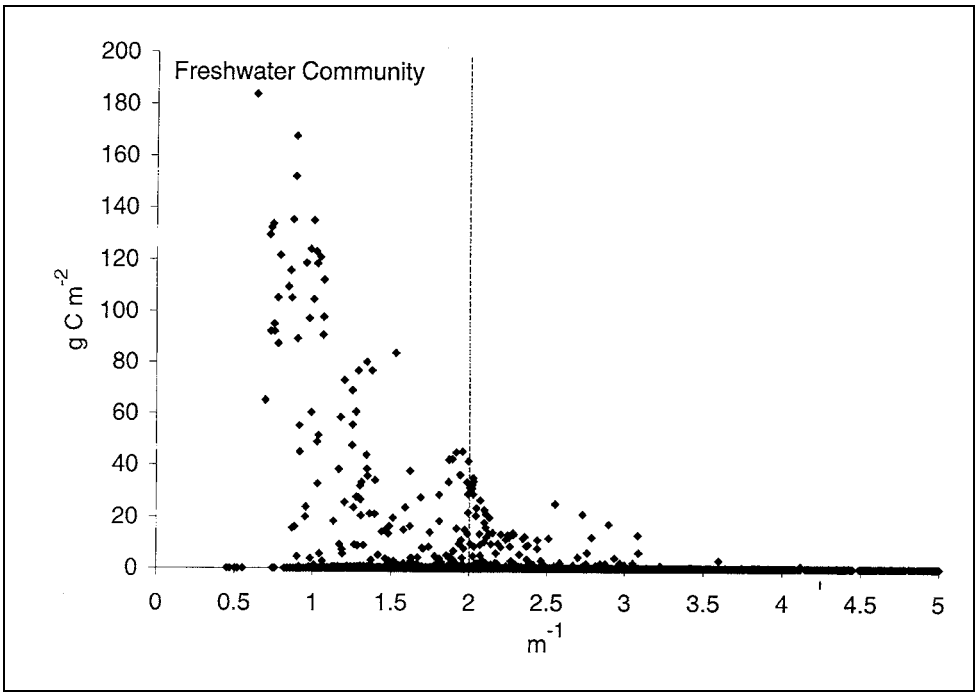


Figure 10. Modeled (mean and interval encompassing 95% of computations) and observed biomass of epiphytes on ZOSTERA. Model results from CBPS CB7.



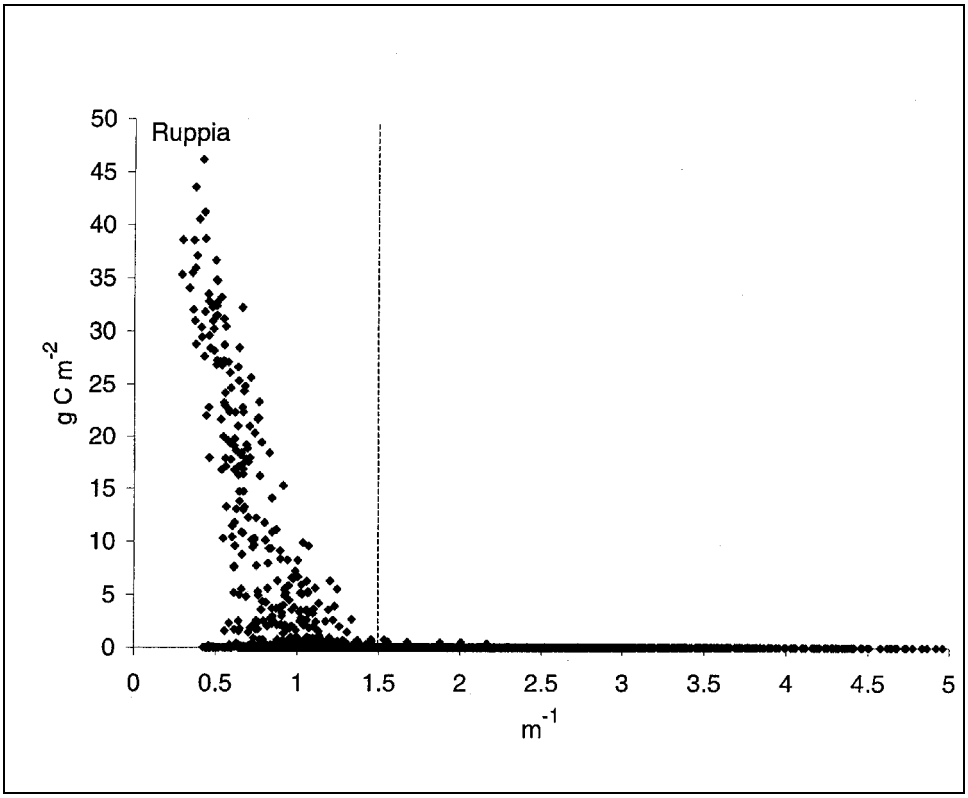


Figure 11. Computed shoot biomass versus light attenuation for (a) FRESHWATER community, (b) RUPPIA, and (c) ZOSTERA. Each point represents seasonal median value in one model cell. Dashed line indicates living-resource criteria for survival at one-meter depth. (Continued).

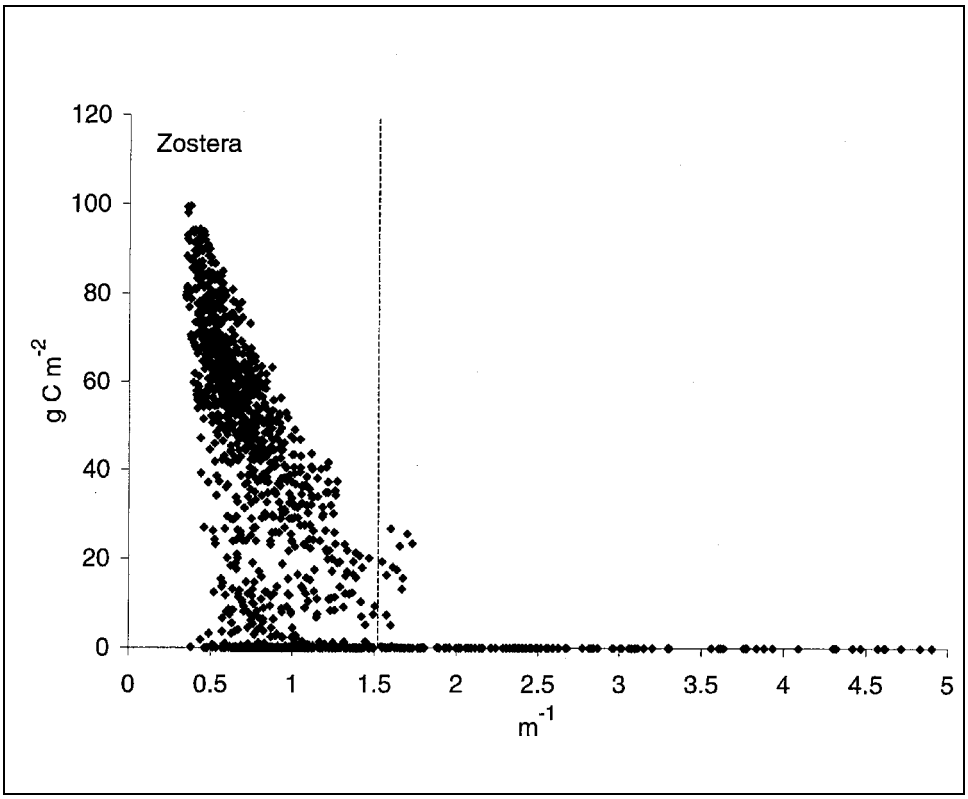
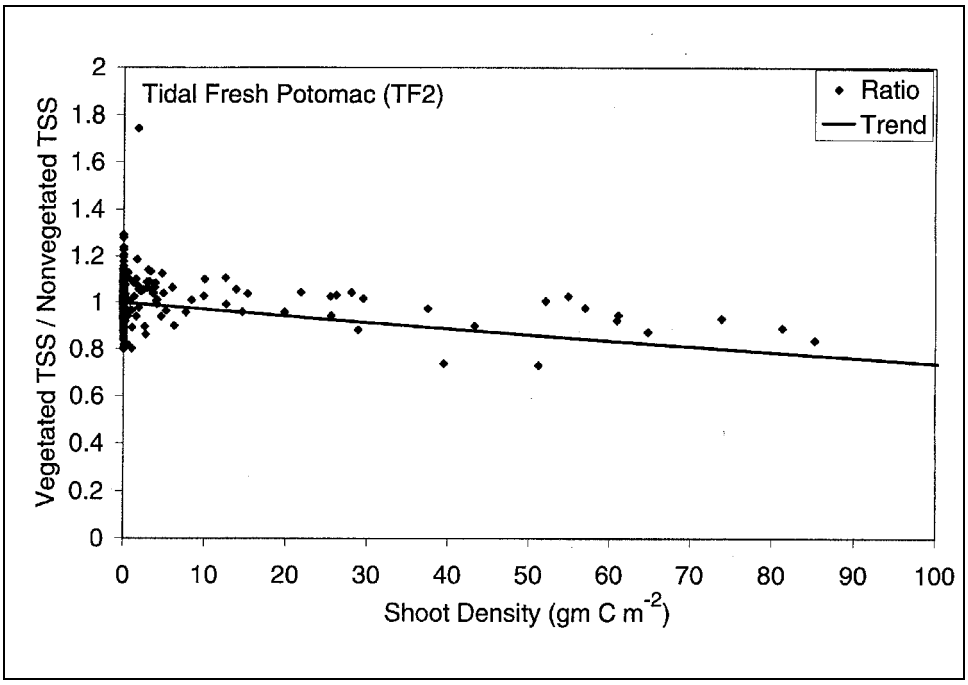


Figure 11. (Concluded).



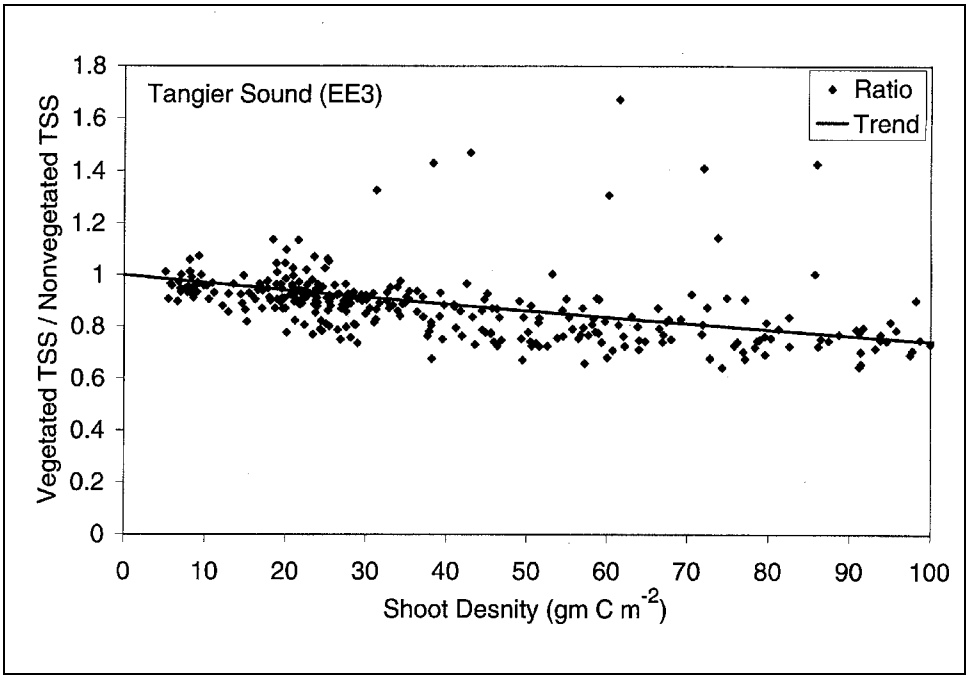


Figure 12. Modeled ratio of suspended solids in vegetated areas to suspended solids in adjacent non-vegetated areas for three CBPS. Trend determined by visual comparison with observations (Continued).

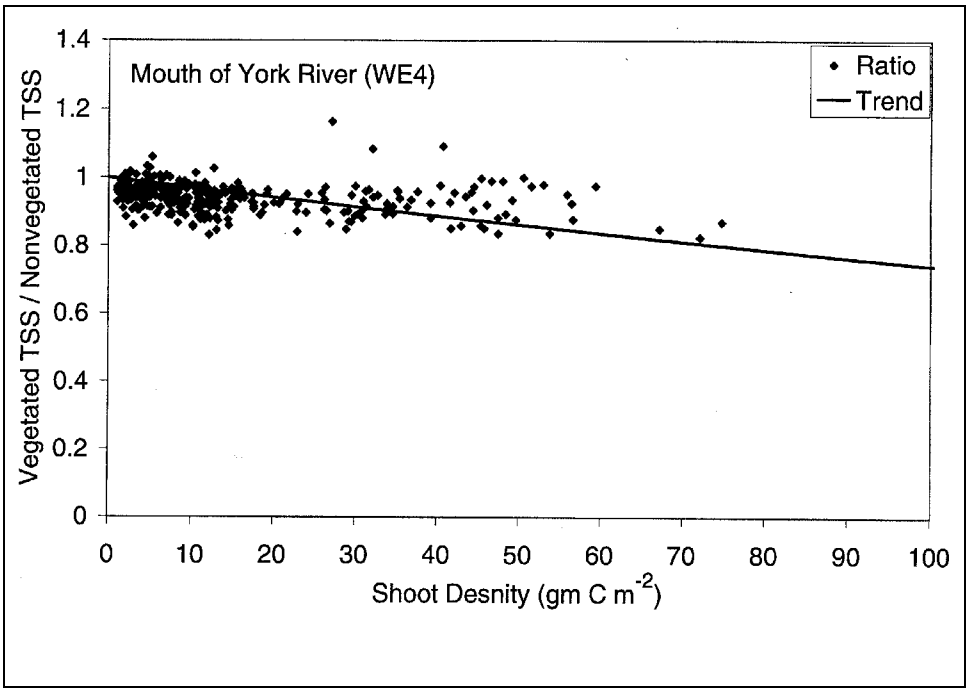


Figure 12. (Concluded).

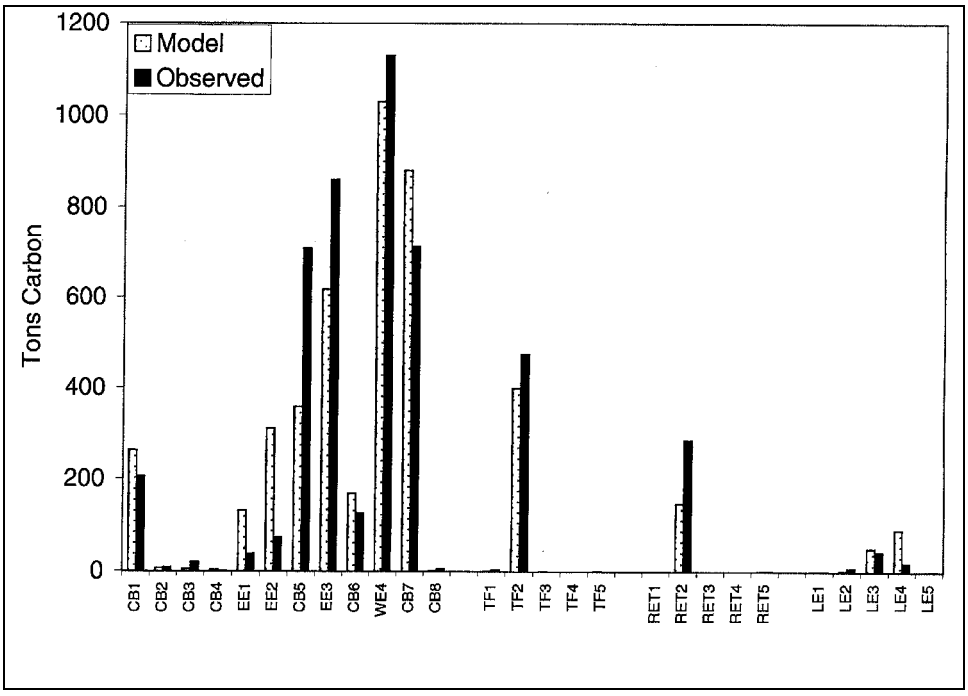


Figure 13. Observed and computed mean abundance, April-October 1985-1994.

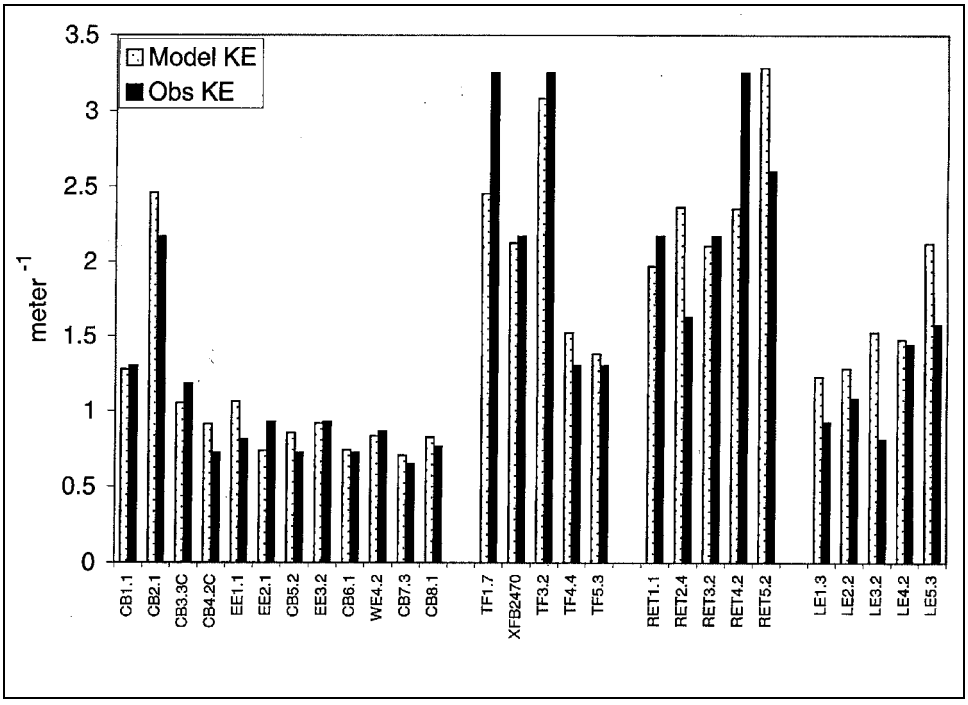


Figure 14. Observed and computed median light attenuation at 27 stations in the bay system, April-October 1985-1994.

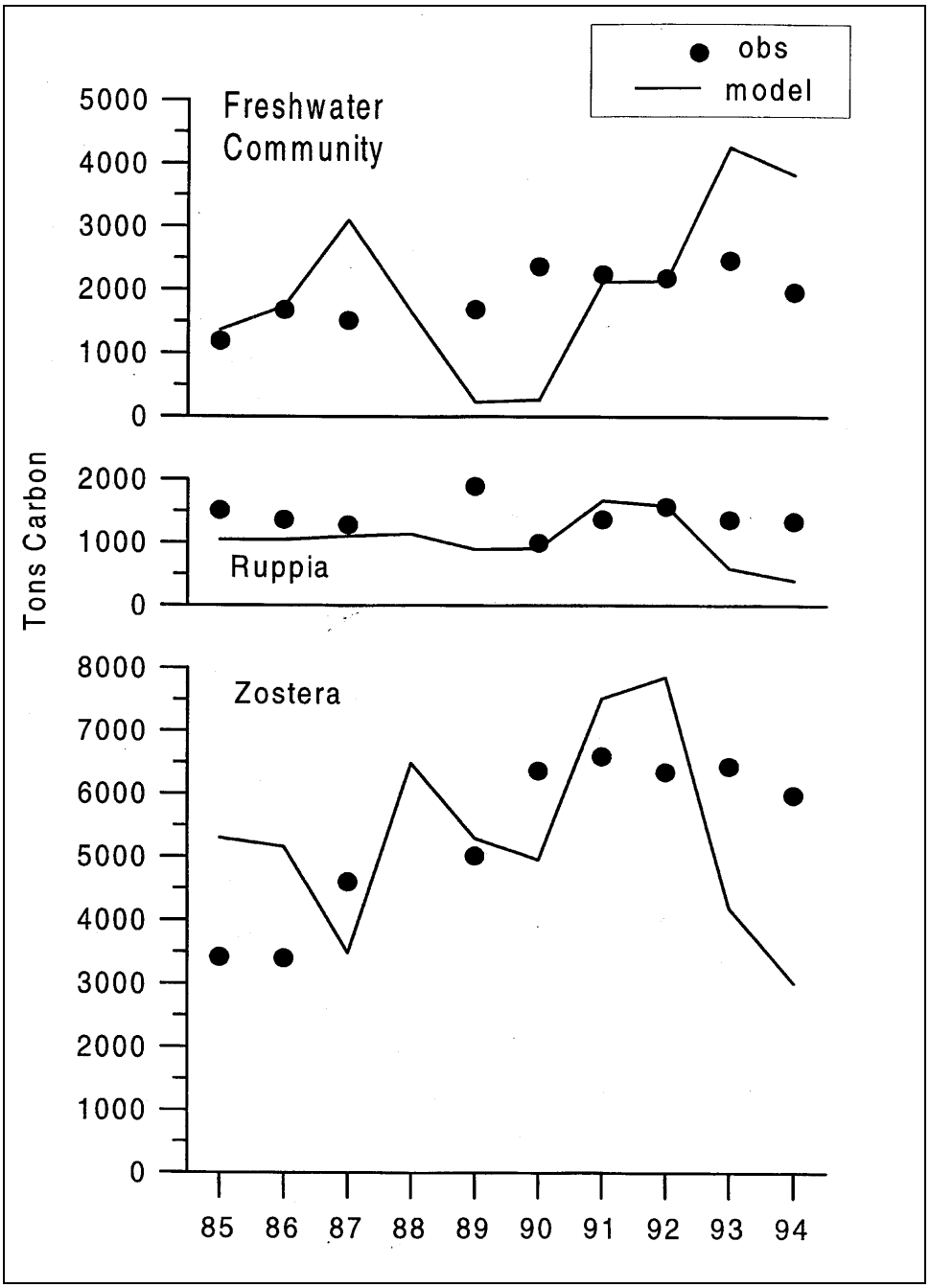


Figure 15. Observed and computed maximum abundance, by community type, 1985-1994.

The Submerged Aquatic Vegetation Input File

The Submerged Aquatic Vegetation (SAV) Input File takes two forms. The primary form, addressed here, provides input to the predictive SAV model. The second form, a vestige of the earliest model code, employs zero-order source and sink terms to simulate SAV materials exchange with the water column. Input for the second option is addressed in a subsequent chapter.

As formulated for Chesapeake Bay, the predictive model simulates an arbitrary number of mutually-exclusive SAV species. Following title information, parameters for each species are input. These are followed by a parameter set applicable to all species. Next, the spatial distribution of the species is detailed. Finally, parameters for the epiphytes are provided.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe zooplankton input deck

Ten text lines head up the SAV Input File. The first four of these are skipped entirely. The next six are title lines are and echoed to the SAV Output File.

Example

```
                        Control file for SAV Module


TITLE CARDS.............................................................
Dec 18, 2001.  Initial set-up on 12,000 cell grid.  Same as Run 162.
Double alpha from SENS162 for three groups.  Leave Potomac alone
Make epiphytes reflect current Group 3
Switch to new distribution of Ruppia that reflects Ken Moore's field data
Decrease epiphyte dry weight to carbon ratio
All grow cells that touch shore = 1m, other grow cells = 2m.
```

Number of Dominant Species

The number of SAV species is specified in a grouping that consists of a blank line, a header line, and an input (//(8X,I8))

Field	Name	Value	Description
1	NDOMSP	Integer	Number of SAV species

Example

```
NDOMSP
     5
```

SAV Species Parameters

Constants

After the number of SAV species is specified, a group of parameters follows for each species. Each parameter group consists of species name, a section of constants and a section of time-varying inputs. A species and parameter set must be specified for each cell in the surface plane of the grid. For various reasons, cells may be unsuited for SAV occurrence. A species named "NO_GROW," with growth, respiration and other parameters set to zero, may be specified for cells with no SAV.

Input for the name (//(8X,A8)) and constants (//(8X,9F8.0) follows a convention of a blank line, a header line, and a line of parameter specification. The first eight columns of each line are skipped by the format statement and may used for identification purposes or left blank.

Field	Name	Value	Description
1	SPNAM	Character	Species name
1	PMSAV	Real	Production at optimum temperature ($g\ C\ g\ DW^{-1}\ d^{-1}$)
2	PRSPSAV	Real	Fraction of photosynthesis consumed in active respiration ($0 \leq PRSPSAV \leq 1$)
3	BMSAV	Real	Basal metabolism of SAV shoots (d^{-1})
4	BMROOT	Real	Basal metabolism of SAV roots (d^{-1})
5	FDOSR	Real	Fraction of photosynthetic oxygen production that provides oxygen to root zone ($0 \leq FDOSR \leq 1$)
6	KHSTOX	Real	Mortality due to sulfide in root zone ($(mol\ H_2S\ m^{-3})^{-1}$)
7	PATCH	Real	Patchiness ($0 \leq PATCH \leq 1$)
1	ACDWSAV	Real	Carbon-to-dry-weight ratio ($g\ C\ g^{-1}\ DW$)
2	ANDWSAV	Real	Nitrogen-to-dry-weight ratio ($g\ N\ g^{-1}\ DW$)
3	APDWSAV	Real	Phosphorus-to-dry-weight ratio ($g\ P\ g^{-1}\ DW$)
1	KHNSH	Real	Half-saturation concentration for nitrogen uptake by shoots ($g\ N\ m^{-3}$)

2	KHNRT	Real	Half-saturation concentration for nitrogen uptake by roots (g N m^{-3})
3	KHPSH	Real	Half-saturation concentration for phosphorus uptake by shoots (g P m^{-3})
4	KHPRT	Real	Half-saturation concentration for phosphorus uptake by roots (g P m^{-3})
1	ALPHSAV	Real	Initial slope of P vs. I curve ((g C g^{-1} DW) (E m^{-2})$^{-1}$)
2	KESAV	Real	Light attenuation by shoots (m^2 g^{-1} C)
3	ACLA	Real	Shoot carbon per unit leaf area (g C m^{-2})
4	ACAN	Real	Constant that relates canopy height to shoot density (m^3 g^{-1} C)
5	BCAN	Real	Exponent in relationship of canopy height to shoot density
1	TRPM	Real	Optimum temperature for production (^oC)
2	TRBMS	Real	Reference temperature for specification of shoot metabolism (^oC)
3	TRBMR	Real	Reference temperature for specification of root metabolism (^oC)
1	KTPS1	Real	Effect of sub-optimal temperature on production ($^oC^{-2}$)
2	KTPS2	Real	Effect of super-optimal temperature on production ($^oC^{-2}$)
3	KTBMS	Real	Effect of temperature on shoot metabolism ($^oC^{-1}$)
4	KTBMR	Real	Effect of temperature on root metabolism ($^oC^{-1}$)

Example

```
  SPNAM
ZOSTERA

   PMSAV PRSPSAV   BMSAV  BMROOT   FDOSR  KHSTOX   PATCH
   0.060    0.10   0.013   0.013   00.10    0.00    0.10

ACDWSAV ANDWSAV APDWSAV
   0.37   0.007 0.00100

  KHNSH   KHNRT   KHPSH   KHPRT
   0.10    0.40   0.020    0.10

ALPHSAV   KESAV    ACLA    ACAN    BCAN
 0.0068   0.045     4.0   0.023    0.53

   TRPM   TRBMS   TRBMR
   22.5    20.0    20.0

  KTPS1   KTPS2   KTBMS   KTBMR
 0.0025   0.010   0.069   0.100
```

Temporally-Varying Parameters

Three SAV parameters may be specified as constants or as temporally-varying. These are sloughing of SAV shoots, the fraction of production routed from shoots to roots, and the transfer of biomass from roots to shoots. The option to vary parameters accounts for physiological processes and environmental cues that are difficult to simulate with continuous, determinate mathematical functions. Each group of the temporally-varying parameters follows the same convention – a blank line, a parameter list, and a line of parameter values. The first parameter list (//8X,2A8) specifies temporally-uniform or varying parameter assignment and determines if input values should be echoed to the output file. For temporally-uniform parameter assignment, the character string 'CONSTANT' should be entered in upper case. Entry of any other string will default to temporally-varying parameter assignment. To print entries to the output file, enter the character string ' ALL'. The second parameter list specifies parameter values (//(8X,3F8.0)). One line of parameter values is required for CONSTANT specification. Otherwise, 366 lines must be entered – one for each day of the year. For convenience, the day may be entered in the first 8 columns. This number is not read into the program. Parameters are understood to be in order starting from day 1.

Field	Name	Value	Description
1	TIMVAR	Character	Temporally uniform (CONSTANT) or varying parameter specification
2	PRINTIT	Character	Print (ALL) or do not print out parameter values
1	SLSAV	Real	Sloughing by SAV shoots (d^{-1})
2	FPSR	Real	Fraction of production routed from shoots to roots ($0 \leq FPSR \leq 1$)
3	TRRS	Real	Transfer of biomass from roots to shoots (d^{-1})

Example

```
      TIMVAR PRINTIT
     VARYING     ALL

        SLSAV    FPSR    TRRS
   1    0.010   0.100   0.000
   2    0.010   0.100   0.000
   3    0.010   0.100   0.000
   4    0.010   0.100   0.000
   5    0.010   0.100   0.000
        .       .       .
        .       .       .
        .       .       .
 361    0.035   0.100   0.000
 362    0.035   0.100   0.000
 363    0.035   0.100   0.000
 364    0.035   0.100   0.000
 365    0.035   0.100   0.000
 366    0.035   0.100   0.000
```

Universal Parameters

The next parameter group consists of constants that apply to all SAV species. Input (//(8X,9F8.0) follows a convention of a blank line, a header line, and a line of parameter specification. The first eight columns of each line are skipped by the format statement and may used for identification purposes or left blank. This parameter group consists largely of parameters that distribute material upon SAV mortality. Mass balance requires the sum of the fractions for each constituent and process to equal unity. No checks exist in the code, however, to enforce this requirement.

Field	Name	Value	Description
1	FNISH	Real	Fraction of shoot nitrogen recycled to dissolved inorganic pool by metabolism ($0 \leq$ FNISH ≤ 1)
2	FNDSH	Real	Fraction of shoot nitrogen recycled to dissolved organic pool by metabolism ($0 \leq$ FNDSH ≤ 1)
3	FNLSH	Real	Fraction of shoot nitrogen recycled to labile particulate pool by metabolism ($0 \leq$ FNLSH ≤ 1)
4	FNRSH	Real	Fraction of shoot nitrogen recycled to refractory particulate pool by metabolism ($0 \leq$ FNRSH ≤ 1)
1	FNISL	Real	Fraction of shoot nitrogen recycled to dissolved inorganic pool by sloughing ($0 \leq$ FNISL ≤ 1)
2	FNDSL	Real	Fraction of shoot nitrogen recycled to dissolved organic pool by sloughing ($0 \leq$ FNDSL ≤ 1)
3	FNLSL	Real	Fraction of shoot nitrogen recycled to labile particulate pool by sloughing ($0 \leq$ FNLSL ≤ 1)
4	FNRSL	Real	Fraction of shoot nitrogen recycled to refractory particulate pool by sloughing ($0 \leq$ FNRSL ≤ 1)
1	FRNSAV1	Real	Fraction of root nitrogen recycled to labile particulate pool by metabolism ($0 \leq$ FRNSAV1 ≤ 1)
2	FRNSAV2	Real	Fraction of root nitrogen recycled to refractory particulate pool by metabolism ($0 \leq$ FRNSAV2 ≤ 1)
3	FRNSAV3	Real	Fraction of root nitrogen recycled to inert particulate pool by metabolism ($0 \leq$ FRNSAV3 ≤ 1)

1	FPISH	Real	Fraction of shoot phosphorus recycled to dissolved inorganic pool by metabolism ($0 \leq$ FPISH ≤ 1)
2	FPDSH	Real	Fraction of shoot phosphorus recycled to dissolved organic pool by metabolism ($0 \leq$ FPDSH ≤ 1)
3	FPLSH	Real	Fraction of shoot phosphorus recycled to labile particulate pool by metabolism ($0 \leq$ FPLSH ≤ 1)
4	FPRSH	Real	Fraction of shoot phosphorus recycled to refractory particulate pool by metabolism ($0 \leq$ FPRSH ≤ 1)
1	FPISL	Real	Fraction of shoot phosphorus recycled to dissolved inorganic pool by sloughing ($0 \leq$ FPISL ≤ 1)
2	FPDSL	Real	Fraction of shoot phosphorus recycled to dissolved organic pool by sloughing ($0 \leq$ FPDSL ≤ 1)
3	FPLSL	Real	Fraction of shoot phosphorus recycled to labile particulate pool by sloughing ($0 \leq$ FPLSL ≤ 1)
4	FPRSL	Real	Fraction of shoot phosphorus recycled to refractory particulate pool by sloughing ($0 \leq$ FPRSL ≤ 1)
1	FRPSAV1	Real	Fraction of root phosphorus recycled to labile particulate pool by metabolism ($0 \leq$ FRPSAV1 ≤ 1)
2	FRPSAV2	Real	Fraction of root phosphorus recycled to refractory particulate pool by metabolism ($0 \leq$ FRPSAV2 ≤ 1)
3	FRPSAV3	Real	Fraction of root phosphorus recycled to inert particulate pool by metabolism ($0 \leq$ FRPSAV3 ≤ 1)
1	KHRSH	Real	Half-saturation concentration for switching shoot respiration from dissolved oxygen consumption to DOC production (g DO m^{-3})
2	FCDSH	Real	Fraction of shoot metabolism released as dissolved organic carbon ($0 \leq$ FCDSH ≤ 1)
1	FCDSL	Real	Fraction of shoot carbon recycled to dissolved organic pool by sloughing ($0 \leq$ FCDSL ≤ 1)
2	FCLSL	Real	Fraction of shoot carbon recycled to labile particulate pool by sloughing ($0 \leq$ FCLSL ≤ 1)

3	FCRSL	Real	Fraction of shoot carbon recycled to refractory particulate pool by sloughing ($0 \leq$ FCRSL ≤ 1)
1	FRCSAV1	Real	Fraction of root carbon recycled to labile particulate pool by metabolism ($0 \leq$ FRCSAV1 ≤ 1)
2	FRCSAV2	Real	Fraction of root carbon recycled to refractory particulate pool by metabolism ($0 \leq$ FRCSAV2 ≤ 1)
3	FRCSAV3	Real	Fraction of root carbon recycled to inert particulate pool by metabolism ($0 \leq$ FRCSAV3 ≤ 1)
1	WSSSAV	Real	Enhanced net settling of fixed solids due to SAV (m^3 g^{-1} C d^{-1})
2	WSLSAV	Real	Enhanced net settling of labile particles due to SAV (m^3 g^{-1} C d^{-1})
3	WSRSAV	Real	Enhanced net settling of refractory particles due to SAV (m^3 g^{-1} C d^{-1})
4	WS1SAV	Real	Enhanced net settling of algal group 1 due to SAV (m^3 g^{-1} C d^{-1})
5	WS2SAV	Real	Enhanced net settling of algal group 2 due to SAV (m^3 g^{-1} C d^{-1})
6	WS3SAV	Real	Enhanced net settling of algal group 3 due to SAV (m^3 g^{-1} C d^{-1})

Example

```
  FNISH   FNDSH   FNLSH   FNRSH
   0.50    0.30    0.15    0.05

  FNISL   FNDSL   FNLSL   FNRSL
   0.00    0.33    0.44    0.23

FRNSAV1 FRNSAV2 FRNSAV3
   0.60    0.30    0.10

  FPISH   FPDSH   FPLSH   FPRSH
   0.50    0.35    0.10    0.05

  FPISL   FPDSL   FPLSL   FPRSL
   0.00    0.33    0.44    0.23

FRPSAV1 FRPSAV2 FRPSAV3
   0.60    0.30    0.10

  KHRSH   FCDSH
    1.0     0.5

  FCDSL   FCLSL   FCRSL
   0.33    0.44    0.23

FRCSAV1 FRCSAV2 FRCSAV3
    0.6     0.3     0.1

 WSSSAV  WSLSAV  WSRSAV  WS1SAV  WS2SAV  WS3SAV  WSUSAV
   0.05    0.05    0.05    0.05    0.05    0.05    0.05
```

Species Distribution

The next portion of the input deck provides species distribution information. A dominant species, corresponding to one of the species named under "SAV Species Parameters," must be specified for each surface cell in the model grid. The user must also specify the mean depth of SAV beds in each surface cell. This latter requirement bridges a gap in resolution between the model cell size and expanse of SAV beds. Model cells are typically several square kilometers in area. The minimum cell depth represented on the Chesapeake Bay grid is 2.1 m. In some locations with plunging bathymetry, the grid adjacent to the shoreline is several cells thick, leading to a depth greater than 2.1 m. SAV beds usually hug the shore and extend to a depth that is less than the average depth represented by a model cell. Consequently, the average depth of the SAV bed is specified independent of the grid depth. Light attenuation, the critical component in SAV production, is calculated based on the depth of the SAV bed.

This portion of the input file consists of a blank line, a line of header information, and one line of parameter values for each surface cell (//(8X,A8,F8.0). Parameters are read in order from cell one to the number of surface cells. The first 8 columns of each line are skipped by the code. These may be used to number input lines for clarity.

Field	Name	Value	Description
1	SAV TYPE	Character	SAV species name
2	BLSAV	Real	Average depth of SAV bed (m)

Example

```
CELL NO SAV TYPE  BLTOAV
      1  VALLISN     1.0   10.00
      2  VALLISN     1.0   10.00
      3   RUPPIA     1.0   10.00
      4  VALLISN     1.0   10.00
      5   RUPPIA     1.0   10.00
            .          .      .
            .          .      .
            .          .      .
   2958  VALLISN     1.0   10.00
   2959  VALLISN     1.0   10.00
   2960  NO_GROW     1.0    0.01
   2961  VALLISN     1.0   10.00
```

Epiphytes

The convention for epiphyte inputs largely follows the convention for SAV Species Parameters. A species name, "EPIPHYTES" is followed by a set of constant parameter values. No spatially varying or cell-specific parameters are required or allowed. Input for the name (//(8X,A8)) and constants (//(8X,9F8.0) follows a convention of a blank line, a header line, and a line of parameter specification. The first eight columns of each line are skipped by the format statement and may used for identification purposes or left blank. A portion of this input section consists of parameters that distribute material upon epiphyte mortality. Mass balance requires the sum of the fractions for each constituent

and process to equal unity. No checks exist in the code, however, to enforce this requirement.

Field	Name	Value	Description
1	EPINAM	Character	Species name
1	PMEPI	Real	Production at optimum temperature (g C g Chl^{-1} d^{-1})
2	PRSPEPI	Real	Fraction of photosynthesis consumed in active respiration ($0 \leq PRSPEPI \leq 1$)
3	BMEPI	Real	Basal metabolism (d^{-1})
4	PREPI	Real	Predation rate (g shoot C g^{-1} epiphyte C d^{-1})
1	CCHLEPI	Real	Carbon-to-chlorophyll ratio (g C g^{-1} Chl)
2	ADWCEPI	Real	Ratio of epiphyte dry weight to viable epiphyte carbon (g DW g^{-1} C)
3	ANCEPI	Real	Nitrogen-to-carbon ratio of viable epiphytes (g N g^{-1} C)
4	APCEPI	Real	Phosphorus-to-carbon ratio of viable epiphytes (g P g^{-1} C)
1	KHNEPI	Real	Half-saturation concentration for nitrogen uptake (g N m^{-3})
2	KHPEPI	Real	Half-saturation concentration for phosphorus uptake (g P m^{-3})
1	ALPHSAV	Real	Initial slope of P vs. I curve ((g C g^{-1} Chl) (E m^{-2})$^{-1}$)
2	KEEPI	Real	Light attenuation by epiphytes (m^2 leaf g^{-1} epiphyte DW)
1	TRPE	Real	Optimum temperature for production (^oC)
2	TRBME	Real	Reference temperature for specification of basal metabolism (^oC)
3	TRPRE	Real	Reference temperature for specification of predation (^oC)
1	KTPE1	Real	Effect of sub-optimal temperature on production ($^oC^{-2}$)
2	KTPE2	Real	Effect of super-optimal temperature on production ($^oC^{-2}$)
3	KTBME	Real	Effect of temperature on metabolism ($^oC^{-1}$)
4	KTPRE	Real	Effect of temperature on predation ($^oC^{-1}$)
1	KHEP	Real	Density at which growth is halved (g epiphyte C g^{-1} shoot C)

1	FNIEPI	Real	Fraction of nitrogen recycled to dissolved inorganic pool by metabolism ($0 \leq$ FNIEPI ≤ 1)
2	FNDEPI	Real	Fraction of nitrogen recycled to dissolved organic pool by metabolism ($0 \leq$ FNDEPI ≤ 1)
3	FNLEPI	Real	Fraction of nitrogen recycled to labile particulate pool by metabolism ($0 \leq$ FNLEPI ≤ 1)
4	FNREPI	Real	Fraction of nitrogen recycled to refractory particulate pool by metabolism ($0 \leq$ FNREPI ≤ 1)
1	FNIPEP	Real	Fraction of nitrogen recycled to dissolved inorganic pool by predation ($0 \leq$ FNIPEP ≤ 1)
2	FNDPEP	Real	Fraction of nitrogen recycled to dissolved organic pool by predation ($0 \leq$ FNDPEP ≤ 1)
3	FNLPEP	Real	Fraction of nitrogen recycled to labile particulate pool by predation ($0 \leq$ FNLPEP ≤ 1)
4	FNRPEP	Real	Fraction of nitrogen recycled to refractory particulate pool by predation ($0 \leq$ FNRPEP ≤ 1)
1	FPIEPI	Real	Fraction of phosphorus recycled to dissolved inorganic pool by metabolism ($0 \leq$ FPIEPI ≤ 1)
2	FPDEPI	Real	Fraction of phosphorus recycled to dissolved organic pool by metabolism ($0 \leq$ FPDEPI ≤ 1)
3	FPLEPI	Real	Fraction of phosphorus recycled to labile particulate pool by metabolism ($0 \leq$ FPLEPI ≤ 1)
4	FPREPI	Real	Fraction of phosphorus recycled to refractory particulate pool by metabolism ($0 \leq$ FPREPI ≤ 1)
1	FPIPEP	Real	Fraction of phosphorus recycled to dissolved inorganic pool by predation ($0 \leq$ FPIPEP ≤ 1)
2	FPDPEP	Real	Fraction of phosphorus recycled to dissolved organic pool by predation ($0 \leq$ FPDPEP ≤ 1)
3	FPLPEP	Real	Fraction of phosphorus recycled to labile particulate pool by predation ($0 \leq$ FPLPEP ≤ 1)

4	FPRPEP	Real	Fraction of phosphorus recycled to refractory particulate pool by predation ($0 \leq$ FPRPEP ≤ 1)
1	KHREP	Real	Half-saturation concentration for switching respiration from dissolved oxygen consumption to DOC production (g DO m^{-3})
2	FCDEPI	Real	Fraction of metabolism released as dissolved organic carbon ($0 \leq$ FCDEPI ≤ 1)
1	FCDPEP	Real	Fraction of carbon recycled to dissolved organic pool by predation ($0 \leq$ FCDPEP ≤ 1)
2	FCLPEP	Real	Fraction of carbon recycled to labile particulate pool by predation ($0 \leq$ FCLPEP ≤ 1)
3	FCRPEP	Real	Fraction of carbon recycled to refractory particulate pool by predation ($0 \leq$ FCRPEP ≤ 1)

Example

```
  EPINAM
EPIPHYTE

   PMEPI PRSPEPI   BMEPI   PREPI
   350.0    0.25   0.020   5.000

 CCHLEPI ADWCEPI  ANCEPI  APCEPI
    75.0    18.0   0.175  0.0175

  KHNEPI  KHPEPI
   0.025  0.0025

 APLHEPI   KEEPI
     8.0    0.06

    TRPE   TRBME   TRPRE
    25.0    20.0    20.0

   KTPE1   KTPE2   KTBME   KTPRE
  0.0035   0.000   0.032   0.069

    KHEP
    0.10

  FNIEPI  FNDEPI  FNLEPI  FNREPI
    0.55    0.20    0.20    0.05

  FNIPEP  FNDPEP  FNLPEP  FNRPEP
    0.40    0.20    0.25    0.15

  FPIEPI  FPDEPI  FPLEPI  FPREPI
    0.75    0.25    0.00    0.05

  FPIPEP  FPDPEP  FPLPEP  FPRPEP
    0.50    0.40    0.07    0.03

   KHREP  FCDEPI
     0.5     0.0

  FCDPEP  FCLPEP  FCRPEP
    0.15    0.65    0.20
```

The Submerged Aquatic Vegetation File

The second form of the Submerged Aquatic Vegetation File provides a means of adding or removing material due to the activity of submerged aquatic vegetation (SAV). In its present configuration, loads are considered for particulate organic matter and for dissolved oxygen. Dissolved nutrients can be added with minor code modifications.

The first three lines in the file are reserved for comments or identification. The next card group lists the total number of cells which contain SAV.

Field	Name	Value	Description
1	SAVLN	Integer	Total number of cells with SAV

EXAMPLE

```
SAVLN
   16
```

The next card group lists the cells which contain SAV.

Field	Name	Value	Description
1-9	SAVLB	Integer	Cells which contain SAV

EXAMPLE

```
SAVLB   SAVLB   SAVLB   SAVLB   SAVLB   SAVLB   SAVLB   SAVLB   SAVLB
    1       3       5       7       8      10      11      13      15
   16      20      21      22      23      24      25
```

The next card group gives the area (square meters) covered by SAV in each of the cells named.

Field	Name	Value	Description
1-9	SAVAREA	Integer	Area covered by SAV

EXAMPLE

```
SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA
   100.    100.    100.    100.    100.    200.    200.    300.   300.
   200.    200.    100.    100.    250.    250.    250.
```

The last card group gives SAV sources or sinks of particulate matter and dissolved oxygen. Units are gm m^{-2} day^{-1}. Sources or sinks may be updated at arbitrary intervals.

Field	Name	Value	Description
1	NXSAV	Integer	Julian day
2	SAVLPOC	Real	Source/sink of labile particulate carbon
3	SAVRPOC	Real	Source/sink of refractory particulate carbon
4	SAVLPON	Real	Source/sink of labile particulate nitrogen
5	SAVRPON	Real	Source/sink of refractory particulate nitrogen
6	SAVLPOP	Real	Source/sink of labile particulate phosphorus
7	SAVRPOP	Real	Source/sink of refractory particulate phosphorus
8	SAVDO	Real	Source/sink of dissolved oxygen

EXAMPLE

NXSAV	SAVLPOC	SAVRPOC	SAVLPON	SAVRPON	SAVLPOP	SAVRPOP	SAVDO
0.0	0.10	0.01	0.001	0.000	0.001	0.00	0.30

Example of Submerged Aquatic Vegetation Input File

```
SUBMERGED AQUATIC VEGETATION FILE FOR 1984
GENERATED OCTOBER 9, 1991.  NO NUTRIENT CONTRIBUTION BY SAV

           SAVLN
              16

           SAVLB   SAVLB   SAVLB   SAVLB   SAVLB   SAVLB   SAVLB   SAVLB  SAVLB
               1       2       7       8      16      17      18      20     21
              27      28      30      39      40      41      42

         SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA SAVAREA
         3.38E+6 1.11E+5 3.05E+6 5.46E+6 2.73E+6 6.24E+6 4.58E+5 7.96E+5 4.58E+4
         2.26E+5 2.48E+5 2.14E+5 3.10E+5 1.29E+6 7.26E+5 1.18E+6

   NXSAV SAVLPOC SAVRPOC SAVLPON SAVRPON SAVLPOP SAVRPOP   SAVDO
   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
 120.000   0.950   0.950   0.000   0.000   0.000   0.000   5.070
 300.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
 364.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
```

Surface Heat Transfer and Irradiance

Introduction

Heat exchange between the water column and the atmosphere is considered proportional to the temperature difference between the water surface and a theoretical equilibrium temperature (Edinger et al. 1974):

$$\Sigma H = KT \cdot (Te - Ts)$$

Equation 1

in which:

ΣH = surface heat exchange (watt m^{-2})
KT = heat exchange coefficient (watt m^{-2} $^oC^{-1}$)
Te = equilibrium temperature (^oC)
Ts = surface temperature (^oC)

The equilibrium temperature and heat exchange coefficient are inputs to the model. They are not calculated within the model. For most practical purposes, the model cannot be operated without these inputs. Therefore we provide here a summary of the formulae for the calculation of equilibrium temperature and heat exchange coefficient and a FORTRAN listing of a program that performs the calculations. The reader is referred to Edinger et al. (1974) for further details.

The equilibrium temperature and heat exchange coefficient can be updated at arbitrary intervals. For applications to coastal waters, we have found daily updates to be sufficient. For Lake Washington, concern about the effects of diurnal heating and cooling of the surface made more frequent updates desirable. The concern was due to potential convectional mixing caused by surface cooling during the night hours. In fact, no connection exists between surface cooling and mixing in the CE-QUAL-ICM model. Convectional mixing is computed in the accompanying hydrodynamic model. Heat exchange parameters were calculated once and used in both models, however, so frequent updates were employed in both models. Meteorological data for calculation of heat exchange was largely

available on an hourly basis but the record was irregular. Consequently, heat exchange parameters were calculated for all available records and averaged into four-hour blocks. Most averages consisted of four records but fewer and, occasionally more, records contributed to some averages.

Heat Budget

Surface heat exchange consists of the following processes:

$$\Sigma H = Hs - Hsr + Han - Hb - He - Hc$$

Equation 2

in which:

Hs = solar radiation (watt m^{-2})
Hsr = reflected solar radiation (watt m^{-2})
Han = net atmospheric radiation (watt m^{-2})
Hb = black-body back-radiation (watt m^{-2})
He = evaporative heat loss (watt m^{-2})
Hc = conductive heat loss (watt m^{-2})

Solar Radiation

Our calculation of solar radiation is derived from Tennessee Valley Authority (1972):

$$Hs = \frac{Io}{r^2} \cdot \sin(\alpha)$$

Equation 3

in which:

Io = solar constant (1395 watt m^{-2})
r = radius vector
α = solar elevation

Radius vector. The radius vector is defined:

$$r = 1 + 0.017 \cdot \cos\left(\frac{2\pi}{365} \cdot (186 - D)\right)$$

Equation 4

in which:

D = day of year ($1 \leq D \leq 365$)

Solar Elevation. The solar elevation is defined (Kirk 1994):

$$\sin(\alpha) = \sin(\phi) \cdot \sin(\delta) - \cos(\phi) \cdot \cos(\delta) \cdot \cos(\tau)$$

Equation 5

in which:

φ= latitude (radians)
δ= declination (radians)

Declination is given by:

$$\delta = 23.45 \cdot \frac{\pi}{180} \cdot \cos\left(\frac{2\pi}{365} \cdot (172 - D) \right)$$

Equation 6

and

$$\tau = \frac{2\pi}{24} \cdot t$$

Equation 7

in which:

t = hours since midnight

Net Solar Radiation. Solar radiation is diminished by cloud cover and further reduced by reflection from the water surface. Reflection is usually 5% to 10% of incoming radiation. In view of the small value of reflection, precise calculation of this factor is not worthwhile. A formula that accounts for cloud cover and reflection is (Ryan and Harleman 1973):

$$Hsn = 0.94 \cdot Hs \cdot \left(1 - 0.65 \cdot C^2\right)$$

Equation 8

in which:

Hsn = net incoming solar radiation (watt m^{-2})
C = cloud cover ($0 \leq C \leq 1$)

Atmospheric Radiation

Radiation emitted by the earth's surface is absorbed by components of the atmosphere and emitted back to the earth and into space. If clouds are present, additional radiation is emitted by water and ice particles at the cloud bottom. Numerous formulae are available for atmospheric radiation. We use

"Swinbank's formula" with modification for a cloudy sky (Tennessee Valley Authority 1972):

$$Ha = 0.937x10^{-5} \cdot (1 + 0.17 \cdot C^2) \cdot \sigma \cdot Tabs^6$$

Equation 9

in which:

Ha = atmospheric radiation (kJ m^{-2} h^{-1})
σ = Stefan-Boltzman constant (2.04x10^{-7} kJ m^{-2} h^{-1} $^oK^{-4}$)
Tabs = absolute air temperature 2 m above water surface (^oK)

Net atmospheric radiation in model units (watt m^{-2} = kJ m^{-2} h^{-1} * 0.278), assuming 3% reflection at the water surface, is:

$$Han = 5.16x10^{-13} \cdot (1 + 0.17 \cdot C^2) \cdot Tabs^6$$

Equation 10

Evaporative Heat Loss

Our formula for evaporative heat loss is obtained from Edinger et al. (1974):

$$He = \beta \cdot (Ts - Td) \cdot f(W)$$

Equation 11

in which:

β = slope of saturated vapor pressure curve (mm Hg $^oC^{-1}$)
Ts = water surface temperature (^oC)
Td = atmospheric dew point temperature (^oC)
f(W) = windspeed function (W m^{-2} mm^{-1} Hg)

Slope of saturated vapor pressure curve. β is defined:

$$\beta = \frac{e_s - e_a}{Ts - Td}$$

Equation 12

in which:

e_s = saturated vapor pressure at water surface temperature (mm Hg)
e_a = vapor pressure in overlying air (mm Hg)

Windspeed Function. A wide variety of windspeed functions is available. We use the formula of Brady, Graves and Geyer (Edinger at al. 1974):

$$f(W) = 9.2 + 0.46 \cdot W^2$$

Equation 13

in which:

W = windspeed measured 7 m above the water surface (m s^{-1})

Surface Heat Transfer and Equilibrium Temperature

Edinger et al. (1974) perform a number of substitutions and approximations to obtain two equations that provide surface heat transfer coefficient and equilibrium temperature through iterative solution:

$$KT = 4.48 + (\beta + 0.47) \cdot f(W) + 0.05 \cdot Ts$$

Equation 14

$$Te = \frac{(Hsn + Han - 306 + (KT - 4.48) \cdot Td^*)}{KT + 0.05 \cdot Td^* - 0.025 \cdot Te}$$

Equation 15

in which:

Td* = modified dew point temperature (^{o}C)

The modified dew point is given as:

$$Td^* = Td + \frac{0.47 \cdot (Ta - Td)}{\beta + 0.47}$$

Equation 16

For these iterations, β is approximated:

$$\beta = 0.35 + 0.015 \cdot \frac{Ts + Td}{2} + 0.0012 \cdot \frac{(Ts + Td)^2}{4}$$

Equation 17

Since the water surface temperature, Ts, is not known when exchange coefficient is calculated external to the model, equilibrium temperature, Te, is substituted in Equations 14 and 17 with little loss of accuracy. A FORTRAN code for evaluating heat transfer coefficient and equilibrium temperature is provided as an appendix to this chapter.

Irradiance

The solar radiation computed via Equation 8, in units of watts per square meter, is suited for heat budget calculations. Solar energy, as watts per square meter (kJ s^{-1} m^{-2}) or langleys per day (g calorie cm^{-2} d^{-1}), has long been used to represent available light in phytoplankton models. Modern measurements of photosynthetic processes employ photosynthetically active radiation (PAR). PAR is the fraction of solar energy within the wavelengths 400 to 700 nm and is commonly measured as quanta or Einstein (1 mole of quanta) per unit area and time. Our present phytoplankton kinetics are based on PAR as E m^{-2} d^{-1}. (This rate should not be confused with daily total irradiance, measured as E m^{-2}.) Ideally, PAR should be measured on-site, but these measurements are not always available. Often, PAR must be derived from observed or computed solar radiation. No exact, universal, conversion between solar radiation and PAR exists although the two must be related (Figure 1). Numerous conversion factors have been published (e.g. Parsons et al. 1984, Kirk 1994) but we have had unsatisfactory results with these. The conversion appears to depend on local influences and/or on instrumentation. Our experience is that the conversion should be based on simultaneous measures of solar radiation and PAR and that the conversion may be site- or instrument-specific.

No measures of solar radiation or PAR were available for the Lake Washington study. We had available long-term measures of PAR at Horn Point MD[1]. We proceeded as follows:

- Compute hourly clear-sky radiation, in watts m^{-2}, at Horn Point for the year 1997. These were computed with Equations 3 – 7.
- Average 24 hourly values into daily values, in watt m^{-2}.
- Account for effects of clouds on daily averages via the relationship expressed in Equation 8.
- Relate daily solar radiation, in watts m^{-2}, to daily total PAR, in E m^{-2}.

Linear regression, forced through zero intercept (Figure 1), indicated PAR = 0.143 * Hs, $R^2 = 0.71$. This relationship was built into the model code to convert calculated solar radiation to PAR.

[1] This record has since been published (Fisher et al. 2003) along with concurrent measures of solar radiation so that a more accurate conversion than the one performed here may be possible.

References

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Fisher, T., Gustafson, A., Radcliffe, G., Sundberg, K., and Stevenson, C. (2003). "A long-term record of photosynthetically available radiation (PAR) and total solar energy at 38.6°N, 78.2°W," *Estuaries*, 26(6), 1450-1460.

Kirk, J. (1994). "Diurnal variation of solar irradiance." *Light & photosynthesis in aquatic ecosystems*. 2nd ed., Cambridge University Press, Cambridge England.

Parsons, T., Takahashi, M., and Hargrave, B. (1984). "The primary formation of particulate materials." *Biological oceanographic processes*. 3rd ed., Pergamon Press, Oxford England.

Ryan, P., and Harleman, D. (1973). "An analytical and experimental study of transient cooling pond behavior," Report No. 161, Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Massachusetts Institute of Technology, Cambridge MA.

Tennessee Valley Authority, (1972). "Heat and mass transfer between a water surface and the atmosphere," Laboratory Report No. 14, Tennessee Valley Authority Division of Water Control Planning Engineering Laboratory, Norris TN.

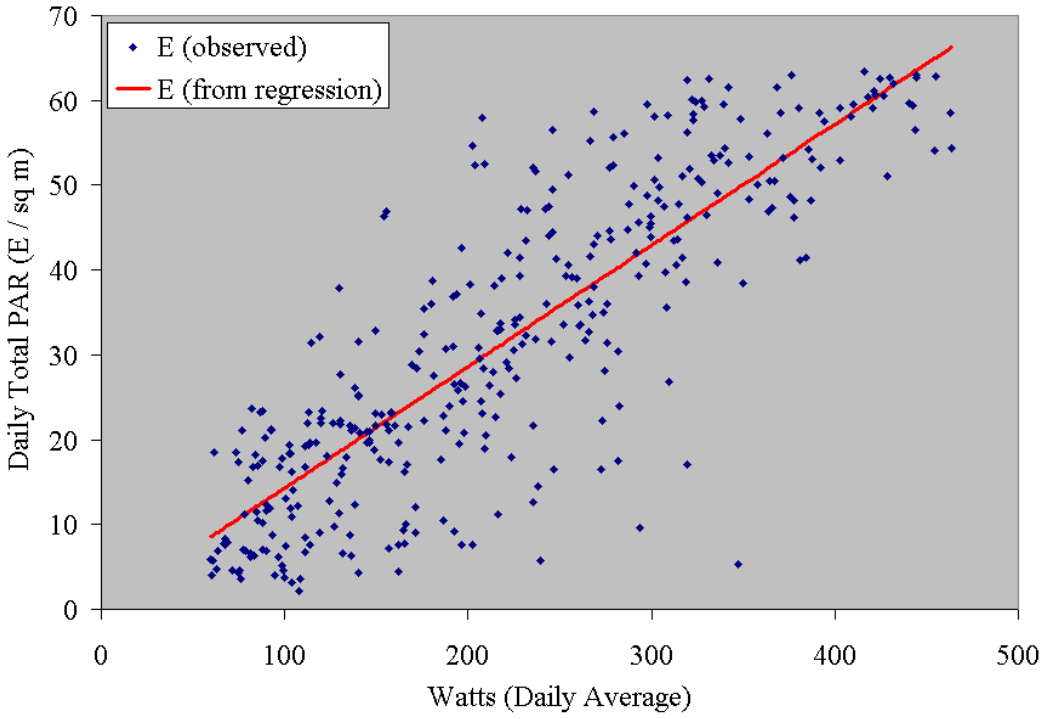

Figure 1. Daily PAR, measured at Horn Point MD, versus calculated solar radiation.

Appendix

```
C A FORTRAN PROGRAM TO COMPUTE SURFACE HEAT EXCHANGE AND EQUILIBRIUM
C TEMPERATURE OCTOBER 15, 2001

C TWO ERRORS CORRECTED FEB 13, 2002

      DATA PI /3.1416/, SOLAR_CONST /1395/

      REAL LATITUDE, KE

      OPEN(10,FILE='heat_exchange.npt',STATUS='OLD')
      OPEN(11,FILE='heat_exchange.opt',STATUS='UNKNOWN')

C CONVERT LATITUDE IN DEGREES, MINUTES, TO RADIANS

      LATITUDE = 2. * PI * (47. + 32./60)/360.

C INITIALIZE DAYS FOR SCAN OF DUPLICATE RECORDS

      DAY_OLD = -999.
      HOUR_OLD = -999.

C INITIAL ESTIMATES OF PARAMETERS NEEDED TO ITERATE KE AND TE

      TENEW = 8.3

 1    READ (10,*,END=999) YEAR, MONTH, DAY, GMT, D_OF_YR, HOUR,
     $  DRY_BULB, WET_BULB, DEW_POINT, WIND, SKY_COVER

C SCAN FOR DUPLICATE RECORDS

      IF (D_OF_YR - DAY_OLD .LT. 0.0007 .AND.
     $  HOUR - HOUR_OLD .LT. 0.0167) GO TO 1

C GET INTEGER DAY FOR OUTPUT

      IDAY = D_OF_YR

C SOLAR RADIATION

      DECL = 23.45*PI/180. * COS(2.*PI*(172. - D_OF_YR)/365.)
      RAD_VEC = 1. + 0.017*COS(2.*PI*(186. - D_OF_YR)/365.)
      TAU = 2.*PI*(HOUR-12.)/24.
      SIN_ALPH = SIN(LATITUDE)*SIN(DECL) +
     $  COS(LATITUDE)*COS(DECL)*COS(TAU)
      HS = SOLAR_CONST*SIN_ALPH/RAD_VEC/RAD_VEC
      HS = MAX(HS,0.)

C CORRECT FOR REFLECTION AND EFFECT OF CLOUDS AS PER R&H PAGE 31
C SKY COVER IS REPORTED IN EIGHTHS.  CONVERT TO FRACTION.

      SKY_COVER = MIN(SKY_COVER,8.)/8.
      HS = 0.94 * HS * (1.-0.65*SKY_COVER*SKY_COVER)

C FRACTIONAL DAYLENGTH AS PER TVA LAB REPORT 14, PAGE 2.10
```

```
      FD = ACOS(-SIN(LATITUDE)*SIN(DECL)/COS(LATITUDE)/COS(DECL))
     $  / PI

C ATMOSPHERIC RADIATION
C USE SWINBANK'S FORMULA AS PER TVA LAB REPORT 14, PAGE 3.18
C THEIR UNITS ARE KJ/M**2/HR.  0.278 CONVERTS TO WATTS/M**2
C ASSUME 3% REFLECTION

      TABS = DRY_BULB +273.15
      HA = 0.937E-5 * 2.0411E-7 * TABS**6 *
     $  (1.+0.17*SKY_COVER*SKY_COVER)
      HA = 0.97 * 0.278 * HA

C TO USE DEWPOINT AS INITIAL GUESS AT TE, UN-COMMENT THE FOLLOWING LINE
C      TENEW = DEW_POINT

C ITERATE UNTIL TE CHANGES BY LESS THAN 0.1 C
C USE FORMULAE IN APPENDIX K OF EDINGER, BRADY, & GEYER

      FW = 9.2 + 0.46 * WIND * WIND

      DO I=1,100

        TE = TENEW
        TM = (TE + DEW_POINT)/2.
        BETA = 0.35 + 0.015 * TM + 0.0012 * TM * TM
        HN = HS + HA

        KE = 4.48 + (BETA + 0.47) * FW + 0.05 * TE
        TDSTAR = DEW_POINT + 0.47 * (DRY_BULB - DEW_POINT) /
     $    (BETA + 0.47)
        TENEW = (HN - 306. + (KE - 4.48) * TDSTAR) /
     $    (KE + 0.05 * TDSTAR - 0.025 * TE)
        IF (ABS(TENEW - TE) .LT. 0.1) GO TO 2

      END DO

 2    WRITE(11,3) IDAY, HOUR, HS, KE, TENEW, WIND, FD
 3    FORMAT(I5, F8.2, F8.1, F8.2, F8.2, F8.1, F8.2)

      DAY_OLD = D_OF_YR
      HOUR_OLD = HOUR
      GO TO 1

 999  END
```

The Meteorological Inputs File

The Meteorological Inputs File contains two sections. These are a title and a section of temporally-varying parameters.

Title Cards

Field	Name	Value	Description
1	Title	Character	Text to describe meteorological inputs file

Two title lines are required to describe the meteorological inputs file. These are not read as variables but are skipped by a FORMAT statement.

Example

```
Meteorological file for Lake Washington 1995
I0 in watts/sq m.  Feb 13, 2002
```

Meteorological Inputs

A blank line and a header line begin the specification of meteorological inputs. Inputs can be updated at arbitrary intervals and must be specified at least twice. The first time is at day zero. If the user wishes to maintain the initial inputs throughout the run, the second specification should be on a Julian day greater than the duration of the model run. If the final specification is on a Julian day less than the run duration, the model code will attempt to open a succeeding meteorological inputs file.

As applied to Lake Washington, all meteorological inputs are held constant until updated. This construction implies that inputs should be updated at intervals that are short relative to the diurnal variation of solar radiation. At present, updates are every four hours. More frequent updates are appropriate. The longest interval should not exceed twelve hours. The fractional daylength, FD, is used to correct the diagnostic output of light limitation. The limitation is reported for daylight hours only. The windspeed, WMS, is used in the reaeration calculation. The format for these inputs is (6F8.0).

Field	Name	Value	Description
1	JDAY	Real	Julian day for parameter update
2	KT	Real	Surface heat transfer coefficient (watts m^{-2} $^oC^{-1}$)
3	TE	Real	Equilibrium temperature (^oC)
4	I0	Real	Solar radiation at water surface (watts m^{-2})
5	FD	Real	Daylight hours as fraction of daylength ($0 \leq FD \leq 1$)
6	WMS	Real	Windspeed (m s^{-1})

Example

JDAY	KT	TE	I0	FD	WMS
0.000	16.73	-6.85	0.0	0.35	3.8
0.167	23.71	-6.39	0.0	0.35	5.5
0.333	24.69	2.21	165.7	0.35	6.0
0.500	22.99	5.92	178.1	0.35	5.5
0.667	25.64	-2.05	3.8	0.35	6.3
0.833	24.43	-4.38	0.0	0.35	6.0
1.000	18.26	-5.62	0.0	0.35	4.3
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
364.000	29.88	7.03	0.0	0.35	5.8
364.167	18.28	5.01	0.0	0.35	3.3
364.333	20.99	10.33	99.4	0.35	3.5
364.500	19.77	12.85	131.3	0.35	3.0
364.667	17.80	6.10	3.6	0.35	3.0
364.833	16.94	5.24	0.0	0.35	2.8

ASCII Output Files

The Snapshot File

The Snapshot File is the primary ASCII output file. Every model run produces a Snapshot File. The first portion of the file lists run specifications input in the Control File. The information listed includes:

Run title and comments.

Input and output file names.

Geometry, time step, and run duration specifications.

Input and output control specifications.

Additional run control specifications.

List of active constituents.

Kinetics parameters.

The balance of the Snapshot File is devoted to ASCII printout of computed concentrations. The printout is an instantaneous "snapshot" of model computations. The times of snapshot output are specified in the Snapshot Control card group in the Control File.

Concentrations are listed for all model cells for all active state variables. Temperature is reported in ^{o}C. Salinity is reported in ppt. All other state variables are reported in g m^{-3}. If the sediment submodel is active, computed concentrations are provided for the sediment as well. All sediment model state variables are reported in mg m^{-3} except benthic stress which has no dimension.

The Snapshot File provides a quick view of model computations. The file is especially useful in diagnosing failed model runs. Contents of the file may also be "cut and pasted" into an initial conditions file or used as plot input. The appropriate binary files are the recommended for these purposes, however.

The Diagnostic File

The Diagnostic File contains information on model performance. The file is especially useful during the model set-up phase and in diagnosing failed model runs. The Diagnostic File is produced when "DIAC = ON" is specified in the Diagnostic Output Control card group in the Control File. Times at which diagnostics are produced are specified in the same group.

Time-Step Diagnostics

The Diagnostic File reports, at user-specified intervals:

Julian days since commencement of model run.

Number of iterations since commencement of model run.

Current time step (seconds).

Average time step since commencement of model run (seconds).

Maximum Courant number at current time step.

Face at which maximum Courant number occurs.

Cell upstream of maximum Courant number face.

Maximum diffusion number at current time step.

Face at which maximum diffusion number occurs.

Cell upstream of maximum diffusion number face.

The Courant number is computed:

$$C = \frac{Q(F)}{V}\Delta t \qquad \textbf{(1)}$$

C = Courant number
Q(F) = volumetric flow at flow face F
V = cell volume upstream of flow face
Δt = time step

The diffusion number is computed:

$$DN = \frac{D \cdot \Delta t \cdot A^2}{V^2} \qquad \textbf{(2)}$$

DN = diffusion number
D = horizontal dispersion coefficient
A = area of flow face F
V = cell volume upstream of flow face
Δt = time step

The Courant and diffusion numbers defined above are analogous to the parameters defined in the chapter entitled “The Conservation of Mass Equation.” The time-step diagnostics aid in the location of model cells and faces that limit the model time step.

Volume-Balance Diagnostics

Cell volumes are initiated whenever a hydrodynamic file is opened. Subsequent to initiation, cell volumes are computed in the water-quality model as a function of volumetric flows specified in the hydrodynamics file. Volume-balance diagnostics compare cell volumes computed in the model with cell volumes produced by the hydrodynamic model. Volume-balance diagnostics are produced when "VBC = ON" is specified on the Miscellaneous Controls card in the Control File.

The Diagnostic File reports, at user-specified intervals:

Total volume of water-quality model grid (m^3).

Difference between water-quality model volume and hydrodynamic model volume (%).

Difference between water-quality model volume and hydrodynamic model volume (m^3).

In addition to global volume statistics, any cells in which the difference in water-quality model volume and hydrodynamic model volume exceeds one-hundred cubic meters are listed.

The volume-balance diagnostics are useful during preparation of the map and hydrodynamics input files. Errors in mapping flow faces or reading hydrodynamics become rapidly apparent in the form of volume imbalances. Volume imbalances also may accrue slowly during a model run. Slow accumulation of volume imbalances usually results from round-off error in the water-quality model. Appropriate variables have been declared as DOUBLE PRECISION in the INCLUDE File to combat roundoff error.

Mass-Balance Diagnostics

The model provides mass-balance summary statistics in the Diagnostic File when "MBLC = ON" is specified in the Mass-Balance Control card group in the Control File. Frequency of statistical output is specified in the same group.

Mass-balance statistics include:

Total mass of each active constituent.

Mass-balance error in water column of nitrogen, phosphorus and carbon (%).

Mass-balance error in sediments of nitrogen, phosphorus and carbon (%).

The mass-balance error is computed:

$$MBE = 100 \cdot \frac{M(t) - M(0) - \sum SS}{M(t) - M(0)} \quad (3)$$

MBE = mass-balance error
M(t) = nutrient mass at time t
M(0) = initial nutrient mass
ΣSS = sum of nutrient sources and sinks since initiation of mass balance

Nutrient masses and the sums of sources and sinks are initialized whenever a hydrodynamic file is opened. When mass balance is perfect, the sum of sources and sinks exactly equals the change in mass since initiation of the balance.

The mass-balance statistic provides a check on linkage between hydrodynamic and water-quality models. The statistic also provides a check on accuracy of computations internal to the water-quality model. Typical mass-balance error at completion of a model run should be $\approx 10^{-2}$%. The user is cautioned that the percent mass-balance error can become unlimited if M(t) approaches M(0). The user is also cautioned that this model option has not been maintained as the model has been updated. Consequently the use of mass-balance diagnostics is not supported.

File Status

Input file names and times at which they are opened are reported in the Diagnostic File.

The Algal Output File

The Algal Output (ALO) File reports parameters input to the phytoplankton component of the eutrophication model. This file is produced whenever one or more algal state variables are active.

The Zooplankton Output File

The Zooplankton Output (ZFO) File reports parameters input to the zooplankton component of the eutrophication model. This file is produced whenever one or more zooplankton state variables are active.

The Benthic Flux Output File

The Benthic Flux Output File is analogous to the Snapshot File. Production of the file is not automatic, however. The file is produced only when "BFOC = ON" is specified on the Miscellaneous Controls card in the Control File.

Contents of the Benthic Flux Output File depend on the specification of benthic fluxes. If the predictive submodel is employed, the file lists input to the submodel including sediment initial conditions. Computed fluxes are provided only in the binary plot files. If user-specified fluxes are employed, the first

portion of Benthic Flux Output File lists the parameters that determine effects of temperature and other factors on the specified fluxes. The balance of the file lists, in ASCII, computed fluxes. All fluxes are in g m^{-2} day^{-1}. The fluxes are output at the same intervals as snapshot printouts.

The Submerged Aquatic Vegetation Output File

The Submerged Aquatic Vegetation Output (SVO) File reports parameters input to the SAV component of the eutrophication model. This file is produced whenever the SAV submodel is active.

The Pathogen and Toxics Output File

The Pathogen and Toxics Output (PTO) File reports parameters input to the pathogen and toxics component of the eutrophication model. This file is produced whenever one or more pathogen and toxics state variables are active.

Binary Output Files

Introduction

The model produces numerous unformatted binary output files. Two of the files, the Initial Conditions Output File and Restart Output File, are produced for use as input in subsequent model runs. The remaining files are the primary output files for model computations. The user must provide programs which read and process model output. Rudimentary post- processors are available from the authors of this guide.

The Initial Conditions Output File

An Initial Conditions Output File is produced at completion of the model run when "ICOC = ON" is specified on the Miscellaneous Controls card in the Control File. The file contains concentrations of all state variables in the water column and sediment. If the steady-state integration option is selected in the Benthic Flux Input File, G3 sediment concentrations at completion of the model run are replaced with estimated steady-state concentrations.

The Initial Conditions Output File from a previous model run is employed as input when "ICIC = BINARY" is specified on the Miscellaneous Controls card in the Control File. Production and employment of binary initial conditions provide a convenient means of looping successive runs while calibrating the model.

The Restart Output File

One or more Restart Output Files are produced when "RSOC = ON" is specified in the Restart Output card group in the Control File. Creation of restart files provides information required to resume a model run after an abnormal termination. The format of the Restart Output File is identical to the Initial Conditions Output File. A restart file can be used to initialize the model by specifying it as a binary initial conditions file in a subsequent model run. Use of restart files provides a “cold start.” The model state variables are initiated based on values in the file but all other information must be input or computed anew.

Restart Output Files are produced at intervals specified in the Restart Output card group. Files are distinguished through a convention provided by the model. The model replaces the last three characters of the Restart Output File name specified in the Control File with the Julian day at which the file is produced.

For example, a file "wqm_rso.123" is produced at Julian day 123 when "wqm_rso.opt" is specified as the Restart Output File name. Julian day is truncated to an integer value. No more than one restart file can be produced per Julian day.

The Plot File

The Plot File contains instantaneous values of concentrations computed within the water column. The Plot File is produced when "PLTC = ON" is specified in the Plot Output Control card group in the Control file. Parameters in the same card group determine the frequency of plot output. Additional output, termed diagnostic information, is produced when "QPLTC = ON" is specified. Sediment-water fluxes and concentrations within the sediments are written to the Plot File when "SPLTC = ON" is specified. Information from the SAV submodel is written to the Plot File when “SAVPLTC=ON” is specified.

Since the Plot File is unformatted, the user must take great care in reading the file into a postprocessing program. A basic guideline is that the READ statements in the postprocessor should conform exactly to the WRITE statements in the model. Correct results require that variable type and array dimensions agree between the model and the postprocessor.

Header information is written to the Plot File once when it is opened. The WRITE statement is:

```
IF (PLOTS) WRITE (PLT) TITLE,NAC,AC,NB,NSPECIES,
     . QUALITY_DIAG,SEDIMENT_DIAG,SAV_PLOTS,
     . ANC1,ANC2,ANC3,APC1,APC2,APC3,ASC1,ASC2,ASC3,
     . ANCSZ,ANCLZ,
     . APCSZ,APCLZ,KADPO4,KADSA,ADWCEPI
```

Variables in the header are summarized in Table 1.

Subsequent information is written to the Plot File repeatedly at intervals specified in the Plot Output Control card group. The WRITE statements are:

```
WRITE (PLT) JDAY,((C1(B,AC(JC)),B=1,NB),JC=1,NAC)

WRITE (PLT) CCHL1,CCHL2,CCHL3

IF (QUALITY_DIAG)   WRITE (PLT) FI1, NL1, PL1, SL1, FI2,
     .         NL2, PL2, SL2, FI3, NL3, PL3, SL3, NPP,
     .         GPP, ASRAT,
     .         NASRAT, CFIX, RESP, KESS, CLSZ, CLLZ, FIB
     .         NLB, PLB, NPPB

IF (SEDIMENT_DIAG)  WRITE (PLT) BENDOC, BENNH4, BENNO3,
     .         BENPO4, BENCOD, BENCH4G, BENCH4A, BENDO,
     .         BENSA,  SSFWS,
     .         PCFWS,  PNFWS,  PPFWS,  PSFWS, CPOC, CPON,
     .         CPOP,
     .         CPIP,  CPOS,  BBM, DFEEDM1S, SFEED
```

```
IF (SAV_PLOTS)      WRITE (PLT) SH, EP, RT, FISH,
     .         NLSAV, PLSAV, FHS, FNSEDSAV, FPSEDSAV, FIEP,
     .         NLEPI,
     .         PLEPI, NPPSH, NPPEPI, WATATN, EPATN
```

Variables in the WRITE statements are listed in Table 1.

Table 1
Variables Written to Plot Output File

Variable	Type	Definition	Units
TITLE	An array with six elements. Each element is CHARACTER*72.	Six title lines from the head of the control file.	
NAC	INTEGER	Number of active constituents	
AC	An INTEGER array with 27 elements.	Sequential number of active constituents. See explanation below.	
NB	INTEGER	Number of cells in model grid	
NSPECIES	INTEGER	Number of suspension feeder species modeled	
QUALITY_DIAG	LOGICAL	.TRUE. if diagnostic information is written to the Plot File. .FALSE. otherwise.	
SEDIMENT_DIAG	LOGICAL	.TRUE. if sediment output is written to the Plot File. .FALSE. otherwise.	
SAV_PLOTS	Logical	.TRUE. if SAV output is written to the Plot File. .FALSE. otherwise.	
ANC1	REAL	Algal group 1 nitrogen-to-carbon ratio	gm N gm^{-1} C
ANC2	REAL	Algal group 2 nitrogen-to-carbon ratio	gm N gm^{-1} C
ANC3	REAL	Algal group 3 nitrogen-to-carbon ratio	gm N gm^{-1} C
APC1	REAL	Algal group 1 phosphorus-to-carbon ratio	gm P gm^{-1} C

APC2	REAL	Algal group 2 phosphorus-to-carbon ratio	gm P gm^{-1} C
APC3	REAL	Algal group 3 phosphorus-to-carbon ratio	gm P gm^{-1} C
ASC1	REAL	Algal group 1 silica-to-carbon ratio	gm Si gm^{-1} C
ASC2	REAL	Algal group 2 silica-to-carbon ratio	gm Si gm^{-1} C
ASC3	REAL	Algal group 3 silica-to-carbon ratio	gm Si gm^{-1} C
ANCSZ	REAL	Microzooplankton nitrogen-to-carbon ratio	gm N gm^{-1} C
ANCLZ	REAL	Mesozooplankton nitrogen-to-carbon ratio	gm N gm^{-1} C
APCSZ	REAL	Microzooplankton phosphorus-to-carbon ratio	gm P gm^{-1} C
APCLZ	REAL	Mesozooplankton phosphorus-to-carbon ratio	gm P gm^{-1} C
KADPO4	REAL	Partition coefficient of sorbed vs. dissolved phosphate	m^3 gm^{-1}
KADSA	REAL	Partition coefficient of sorbed vs. dissolved silica	m^3 gm^{-1}
ADWCEPI	REAL	Epiphyte dry weight-to-carbon ratio	gm DW gm^{-1} C
JDAY	REAL	Julian day elapsed since beginning of run	day
C1	A REAL array dimensioned (0:NBP,NCP). NBP=maximum number of cells. NCP= maximum number of state variables. These are assigned in the INCLUDE file.	C1 is the array containing computed concentrations. See explanation below.	See explanation below
NB	INTEGER	Number of cells in grid	
NAC	INTEGER	Number of active constituents	
CCHL1	A REAL array dimensioned (NBP)	Algal group 1 carbon-to-chlorophyll ratio	gm C gm^{-1} chl
CCHL2	A REAL array dimensioned (NBP)	Algal group 2 carbon-to-chlorophyll ratio	gm C gm^{-1} chl

CCHL3	A REAL array dimensioned (NBP)	Algal group 3 carbon-to-chlorophyll ratio	gm C gm^{-1} chl
FI1	A REAL array dimensioned (NBP)	Light limitation on algal group 1	$0 \leq FI1 \leq 1$
NL1	A REAL array dimensioned (NBP)	Nitrogen limitation on algal group 1	$0 \leq NL1 \leq 1$
PL1	A REAL array dimensioned (NBP)	Phosphorus limitation on algal group 1	$0 \leq PL1 \leq 1$
SL1	A REAL array dimensioned (NBP)	Silica limitation on algal group 1	$0 \leq SL1 \leq 1$
FI2	A REAL array dimensioned (NBP)	Light limitation on algal group 2	$0 \leq FI2 \leq 1$
NL2	A REAL array dimensioned (NBP)	Nitrogen limitation on algal group 2	$0 \leq NL2 \leq 1$
PL2	A REAL array dimensioned (NBP)	Phosphorus limitation on algal group 2	$0 \leq PL2 \leq 1$
SL2	A REAL array dimensioned (NBP)	Silica limitation on algal group 2	$0 \leq SL2 \leq 1$
FI3	A REAL array dimensioned (NBP)	Light limitation on algal group 3	$0 \leq FI3 \leq 1$
NL3	A REAL array dimensioned (NBP)	Nitrogen limitation on algal group 3	$0 \leq NL3 \leq 1$
PL3	A REAL array dimensioned (NBP)	Phosphorus limitation on algal group 3	$0 \leq PL3 \leq 1$
SL3	A REAL array dimensioned (NBP)	Silica limitation on algal group 3	$0 \leq SL3 \leq 1$
NPP	A REAL array dimensioned (NBP)	Algal net primary production	gm C m^{-2} day^{-1}
GPP	A REAL array dimensioned (NBP)	Algal gross primary production	gm C m^{-2} day^{-1}
ASRAT	A REAL array dimensioned (NSBP)	Instantaneous gross assimilation ratio including effects of nutrient limitation	gm C gm^{-1} Chl d^{-1}

NASRAT	A REAL array dimensioned (NSBP)	Instantaneous net assimilation ratio including effects of nutrient and light limitations	gm C gm^{-1} Chl d^{-1}
CFIX	A REAL array dimensioned (NSBP)	Instantaneous gross carbon fixation including effects of nutrient limitation	g C m^{-3} d^{-1}
RESP	A REAL array dimensioned (NBP)	Total oxygen consumption in water column	gm DO m^{-3}
KESS	A REAL array dimensioned (NBP)	Llight extinction including algal self shading	m^{-1}
CLSZ	A REAL array dimensioned (NBP)	Carbon limitation to microzooplankton growth	$0 \leq CLSZ \leq 1$
CLLZ	A REAL array dimensioned (NBP)	Carbon limitation to mesoozooplankton growth	$0 \leq CLLZ \leq 1$
FIB	A REAL array dimensioned (NSBP)	Light limitation on benthic algae	$0 \leq FIB \leq 1$
NLB	A REAL array dimensioned (NSBP)	Nitrogen limitation on benthic algae	$0 \leq NLB \leq 1$
PLB	A REAL array dimensioned (NSBP)	Phosphorus limitation on benthic algae	$0 \leq PLB \leq 1$
NPPB	A REAL array dimensioned (NSBP)	Benthic algal net primary production	gm C m^{-2} day^{-1}
BENDOC	A REAL array dimensioned (NSBP)	Sediment-water dissolved organic carbon flux	gm C m^{-2} day^{-1}
BENNH4	A REAL array dimensioned (NSBP)	Sediment-water ammonium flux.	gm N m^{-2} day^{-1}
BENNO3	A REAL array dimensioned (NSBP)	Sediment-water nitrate flux.	gm N m^{-2} day^{-1}
BENPO4	A REAL array dimensioned (NSBP)	Sediment-water phosphate flux.	gm P m^{-2} day^{-1}
BENCOD	A REAL array dimensioned (NSBP)	Sediment-water COD flux.	gm O_2 equivalents m^{-2} day^{-1}
BENCH4G	A REAL array dimensioned (NSBP)	Sediment-water gaseous methane flux	gm O_2 equivalents m^{-2} day^{-1}
BENCH4A	A REAL array dimensioned (NSBP)	Sediment-water aqueous methane flux	gm O_2 equivalents m^{-2} day^{-1}

BENDO	A REAL array dimensioned (NSBP)	Sediment oxygen demand	gm O_2 m^{-2} day^{-1}
BENSA	A REAL array dimensioned (NSBP)	Sediment-water silica flux.	gm Si m^{-2} day^{-1}
SSFWS	A REAL array dimensioned (NSBP)	Suspended solids flux from water to sediment.	gm m^{-2} day^{-1}
PCFWS	A REAL array dimensioned (NSBP)	Particulate carbon flux from water to sediment	gm C m^{-2} day^{-1}
PNFWS	A REAL array dimensioned (NSBP)	Particulate nitrogen flux from water to sediment	gm N m^{-2} day^{-1}
PPFWS	A REAL array dimensioned (NSBP)	Particulate phosphorus flux from water to sediment	gm P m^{-2} day^{-1}
PSFWS	A REAL array dimensioned (NSBP)	Particulate silica flux from water to sediment	gm Si m^{-2} day^{-1}
CPOC	A REAL array dimensioned (NSBP,3)	Particulate organic carbon concentration in sediment. Second subscript denotes G1, G2, G3 fractions respectively	mg C m^{-3}
CPON	A REAL array dimensioned (NSBP,3)	Particulate organic nitrogen concentration in sediment. Second subscript denotes G1, G2, G3 fractions respectively	mg N m^{-3}
CPOP	A REAL array dimensioned (NSBP,3)	Particulate organic phosphorus concentration in sediment. Second subscript denotes G1, G2, G3 fractions respectively	mg P m^{-3}
CPIP	A REAL array dimensioned (NSBP)	Particulate inorganic phosphorus concentration in sediment	mg P m^{-3}
CPOS	A REAL array dimensioned (NSBP)	Particulate biogenic silica concentration in sediment	mg Si^{-3}
BBM	A REAL array dimensioned (NSBP)	Benthic algal biomass	gm C m^{-2}
DFEEDM1S	A REAL array dimensioned (NSBP)	Deposit feeder biomass	mg C m^{-2}

SFEED	A REAL array dimensioned (NSBP,NSSFP)	Suspension feeder biomass. Second subscript denotes individual species.	mg C m^{-2}
SH	A REAL array dimensioned (NSBP)	SAV shoot density	g C m^{-2}
EP	A REAL array dimensioned (NSBP)	Epiphyte density	g epiphyte C g^{-1} shoot carbon
RT	A REAL array dimensioned (NSBP)	SAV root density	g C m^{-2}
FISH	A REAL array dimensioned (NSBP)	Light limitation on SAV	$0 \leq FISH \leq 1$
NLSAV	A REAL array dimensioned (NSBP)	Nitrogen limitation on SAV	$0 \leq NLSAV \leq 1$
PLSAV	A REAL array dimensioned (NSBP)	Phosphorus limitation on SAV	$0 \leq PLSAV \leq 1$
FHS	A REAL array dimensioned (NSBP)	Sulfide toxicity effect on SAV	$0 \leq FHS \leq 1$
FNSEDSAV	A REAL array dimensioned (NSBP)	Fraction of SAV nitrogen uptake obtained from sediments	$0 \leq FNSEDSAV \leq 1$
FPSEDSAV	A REAL array dimensioned (NSBP)	Fraction of SAV phosphorus uptake obtained from sediments	$0 \leq FPSEDSAV \leq 1$
FIEP	A REAL array dimensioned (NSBP)	Light limitation on epiphytes	$0 \leq FIEP \leq 1$
NLEPI	A REAL array dimensioned (NSBP)	Nitrogen limitation on epiphytes	$0 \leq NLEP \leq 1$
PLEPI	A REAL array dimensioned (NSBP)	Phosphorus limitation on epiphytes	$0 \leq PLEP \leq 1$
NPPSH	A REAL array dimensioned (NSBP)	Instantaneous SAV net production	g C m^{-2} d^{-1}
NPPEPI	A REAL array dimensioned (NSBP)	Instantaneous epiphyte net production	g epiphyte C g^{-1} shoot carbon d^{-1}
WATATN	A REAL array dimensioned (NSBP)	Fraction of surface irradiance remaining at SAV canopy	$0 \leq WATATN \leq 1$
EPATN	A REAL array dimensioned (NSBP)	Fraction of irradiance that passes through epiphyte layer	$0 \leq EPATN \leq 1$

Sequencing of Active Constituents

In its present configuration, the model computes a maximum of 27 state

variables or constituents. Each constituent is assigned an invariant serial number. These are listed in Table 2.

Table 2
State Variables and Serial Numbers

Serial Number	Variable	Serial Number	Variable
1	Temperature	14	Dissolved organic nitrogen
2	Salinity	15	Labile particulate organic nitrogen
3	Inorganic suspended solids	16	Refractory particulate organic nitrogen
4	Cyanobacteria	17	Total phosphate
5	Diatoms	18	Dissolved organic phosphorus
6	Green algae	19	Labile particulate organic phosphorus
7	Microzooplankton	20	Refractory particulate organic phosphorus
8	Mesozooplankton	21	Chemical oxygen demand
9	Dissolved Organic Carbon	22	Dissolved oxygen
10	Labile Particulate Organic Carbon	23	Particulate biogenic silica
11	Refractory Particulate Organic Carbon	24	Dissolved silica
12	Ammonium	25	Pathogen
13	Nitrate+nitrite	26	Toxic 1
		27	Toxic 2

The C1 array contains only the state variables that are "active" as specified in the Active Constituents card group in the Control File. The active variables are indicated by placing their serial numbers in array AC. The total number of active constituents is indicated by variable NAC. For example, if temperature, salinity, and dissolved oxygen are the only active state variables,

NAC = 3. The first three elements of array AC are 1, 2, 22. The remaining elements of AC are 0. Vector C1(B,1) contains temperature predictions. Vector C1(B,2) contains salinity predictions. Vector C1(B,3) contains dissolved oxygen predictions.

The Average Plot File

The Average Plot File contains average values of concentrations computed within the water column. The Average Plot File is produced when "APLC = ON" is specified in the Average Plot Output Control card group in the Control file. Parameters in the same card group determine the interval over which model computations are averaged. Averages of diagnostic information, sediment-water fluxes, and SAV computations are produced when "QPLTC = ON," "SPLTC = ON," and "SAVPLTC=ON" are specified, respectively

Since the Average Plot File is unformatted, the user must take great care in reading the file into a postprocessing program. A basic guideline is that the READ statements in the postprocessor should conform exactly to the WRITE statements in the model. Correct results require that variable type and array dimensions agree between the model and the postprocessor.

Header information is written to the Average Plot File once when it is opened. The WRITE statements are:

```
WRITE (APL) TITLE,NAC,AC,NB,NSPECIES,QUALITY_DIAG,
     .   SEDIMENT_DIAG,SAV_PLOTS,
     .    ANC1,ANC2,ANC3,APC1,APC2,APC3,ASC1,ASC2,ASC3,
     .    ANCSZ,ANCLZ,
     .    APCSZ,APCLZ,KADPO4,KADSA,ADWCEPI

WRITE (APL) NSB,V1,SFA,PATCH
```

The first WRITE statement is identical to the statement that initiates the Plot File. Variables in the second WRITE statement are summarized in Table 3.

Subsequent information is written to the Average Plot File repeatedly at intervals specified in the Average Plot Output Control card group. The WRITE statements are:

```
WRITE (APL) JDAY,((AC1(B,AC(JC)),B=1,NB),JC=1,NAC)

WRITE (APL) ACCHL1,ACCHL2,ACCHL3

WRITE (APL) AFI1, ANL1, APL1, ASL1, AFI2, ANL2, APL2,
     .  ASL2, AFI3, ANL3, APL3, ASL3, ANPP, AGPP, AASRAT,
     .  ANASRAT, ACFIX, ARESP, AKE, ACLSZ,ACLLZ,AFIB,
     .  ANLB, APLB, ANPPB

WRITE (APL) ABENDOC, ABENNH4, ABENNO3, ABENPO4, ABENCOD,
     .  ABENCH4G, ABENCH4A,
     .  ABENDO,  ABENSA,  ASSFWS,  APCFWS,  APNFWS,
     .  APPFWS,  APSFWS,  ACPOC,   ACPON,   ACPOP,
```

```
     .  ACPIP,   ACPOS,   ABBM,    ABLITE,  ADFEED,
     .  ASFEED

WRITE (APL) ASH, AEP, ART, AFISH, ANLSAV,
     $ APLSAV, AFHS,
     $ AFNSED, AFPSED, AFIEP, ANLEPI, APLEPI, ANPPSH,
     $ ANPPEP,
     $ AWATATN,AEPATN
```

Quantities written to the Average Plot File are analogous to variables written to the Plot File and listed in Table 1. The letter "A" at the beginning of the variable name indicates the variables are averaged before output.

Table 3
Variables Written to Average Plot File

Variable	Type	Definition	Units
NSB	INTEGER	Number of surface cells in grid	
V1	A REAL*8 array dimensioned (0:NBP). NBP=maximum number of cells assigned in the INCLUDE file.	Volume of model cell	m^3
SFA	A REAL array dimensioned (NSBP). NSBP=maximum number of surface cells assigned in the INCLUDE file.	Surface area of model cell	m^2
PATCH	A REAL array dimensioned (NSBP).	SAV patchiness	$0 \leq PATCH \leq 1$

The Transportation Flux File

The Transportation Flux File contains computed transport of carbon, nitrogen, and phosphorus at all model flow faces. Computed transport includes the effects of advection, diffusion, and settling. The flux algorithm installed in the model code computes transport of all state variables but these are summarized into substances of most interest prior to output. Positive flux is defined in the positive flow direction, as specified in the Map File. Horizontal fluxes are positive from left to right. Vertical fluxes are positive upwards.

Transport fluxes are output when "TFLC = ON" is specified in the Transport Flux Output Control card group in the Control File. Transport fluxes are averaged over user-specified intervals. The averaging interval is also specified in the Transport Flux Output Control card group.

Header information is written to the Transportation Flux File once when it is opened. The WRITE statement is:

```
WRITE (TFL) TITLE,NQF
```

Variables in the header are summarized in Table 4.

Subsequent information is written to the Transportation Flux File repeatedly at intervals specified in the Transport Flux Output Control card group. The WRITE statement is:

```
WRITE (TFL) JDAY,AFLUX
```

Variables in the WRITE statement are summarized in Table 4.

Table 4
Variables Written to Transportation Flux File

Variable	Type	Definition	Units
TITLE	An array with six elements. Each element is CHARACTER*72.	Six title lines from the head of the Control File	
NQF	INTEGER	Number of flow faces in grid	
JDAY	REAL	Julian day elapsed since beginning of run	day
AFLUX	A REAL array dimensioned (NQFP,16). NQFP = maximum number of flow faces assigned in the INCLUDE file.	Flux of 16 forms of individual and summary quantities. See explanation below.	gm sec^{-1} except pathogen in organisms sec^{-1}

Sequencing of Transportation Fluxes

Sixteen forms of carbon, nitrogen, phosphorus, solids, pathogen, and toxics are output. Each form occupies one vector of the array AFLUX. The first subscript of AFLUX indicates flow face number in the grid. The second subscript indicates the flux. A key to these fluxes is presented in Table 5.

Table 5
Contents of AFLUX Array

Vector	Contents	Vector	Contents
1	Particulate organic carbon	9	Total phosphate
2	Dissolved organic carbon	10	Particulate organic phosphorus
3	Total organic carbon	11	Not implemented
4	Dissolved organic nitrogen	12	Total phosphorus

5	Dissolved inorganic nitrogen	13	Suspended solids
6	Particulate organic nitrogen	14	Pathogen
7	Total nitrogen	15	Toxic 1
8	Dissolved organic phosphorus	16	Toxic 2

The Mass-Balance File

The Mass-Balance File is a complement to the Transportation Flux file. The Mass-Balance File contains the sources and sinks of total carbon, nitrogen, and phosphorus for each water-column and sediment cell. The mass balance enumerates external loading, sediment-water fluxes, and loss of total substance through reactions including respiration and denitrification.

The Mass-Balance file was inaugurated with the first implementation of the model. The accuracy of the algorithms has not been checked as the model has been updated. The description below is accurate. However, the use of the Mass-Balance file is not supported.

Mass balances are output when "MBLC = ON" is specified in the Mass Balance Output Control card group in the Control File. Mass balances are averaged over user-specified intervals. The averaging interval is also specified in the Mass Balance Output Control card group.

Header information is written to the Mass-Balance File once when it is opened. The WRITE statement is:

```
WRITE (MBL) NSB,NB,NHQF,SBN,BBN
```

Variables in the WRITE statement are summarized in Table 6.

Subsequent information is written to the Mass-Balance File repeatedly at intervals specified in the Mass Balance Output Control card group. The WRITE statements are:

```
WRITE (MBL) JDAY

WRITE (MBL) DLWCKMNB,BENFLXPNB,BENFLXDNB,S1FLXNB,S2FLXNB,
     .    S3FLXNB,ATMFLXNB

WRITE (MBL) BENFLXPPB,BENFLXDPB,S1FLXPB,S2FLXPB,S3FLXPB,
     .    ATMFLXPB

WRITE (MBL) DLWCKMCB,BENFLXPCB,S1FLXCB,S2FLXCB,S3FLXCB

WRITE (MBL) DLSEDKNB,BURIALFLXNB

WRITE (MBL) BURIALFLXPB

WRITE (MBL) DLSEDKCB,BURIALFLXCB
```

Variables in the WRITE statements are summarized in Table 6.

Table 6
Variables Written to Mass-Balance File

Variable	Type	Definition	Units
NSB	INTEGER	Number of surface cells in model grid	
NB	INTEGER	Number of cells in model grid	
NHQF	INTEGER	Number of horizontal flow faces in model grid	
SBN	An INTEGER array dimensioned (NSBP). NSBP = maximum number of surface cells. NSBP is assigned in INCLUDE file.	An array of surface cell numbers. See explanation below.	
BBN	An INTEGER array dimensioned (NSBP)	An array of bottom cell numbers. See explanation below.	
JDAY	REAL	Julian day elapsed since beginning of run	day
DLWCKMNB	A REAL array dimensioned (NBP). NBP = maximum number of grid cells. NBP is assigned in INCLUDE file.	Total nitrogen source or sink in cell due to kinetics in water column. The sole term is loss due to denitrification.	kg day^{-1}
BENFLXPNB	A REAL array dimensioned (NSBP)	Total particulate nitrogen flux from water to sediment cell. This a negative number when material is input to sediment.	kg day^{-1}
BENFLXDNB	A REAL array dimensioned (NSBP)	Total dissolved nitrogen flux from water to sediment cell. This a negative number when material is input to sediment.	kg day^{-1}
S1FLXNB	A REAL array dimensioned (NBP)	Total nitrogen load to cell from External Load File 1.	kg day^{-1}
S2FLXNB	A REAL array dimensioned (NBP)	Total nitrogen load to cell from External Load File 2.	kg day^{-1}
S3FLXNB	A REAL array dimensioned (NBP)	Total nitrogen load to cell from External Load File 3.	kg day^{-1}
ATMFLXNB	A REAL array dimensioned (NSBP)	Total atmospheric nitrogen load to model cell.	kg day^{-1}

BENFLXPPB	A REAL array dimensioned (NSBP)	Total particulate phosphorus flux from water to sediment cell. This a negative number when material is input to sediment.	kg day^{-1}
BENFLXDPB	A REAL array dimensioned (NSBP)	Total dissolved phosphorus flux from water to sediment cell. This a negative number when material is input to sediment.	kg day^{-1}
S1FLXPB	A REAL array dimensioned (NBP)	Total phosphorus load to cell from External Load File 1.	kg day^{-1}
S2FLXPB	A REAL array dimensioned (NBP)	Total phosphorus load to cell from External Load File 2.	kg day^{-1}
S3FLXPB	A REAL array dimensioned (NBP)	Total phosphorus load to cell from External Load File 3.	kg day^{-1}
ATMFLXPB	A REAL array dimensioned (NSBP)	Total atmospheric phosphorus load to model cell.	kg day^{-1}
DLWCKMCB	A REAL array dimensioned (NBP)	Total carbon source or sink in cell due to kinetics in water column. Terms include primary production and respiration.	kg day^{-1}
BENFLXPCB	A REAL array dimensioned (NSBP)	Total particulate carbon flux from water to sediment cell. This a negative number when material is input to sediment.	kg day^{-1}
S1FLXCB	A REAL array dimensioned (NBP)	Total carbon load to cell from External Load File 1.	kg day^{-1}
S2FLXCB	A REAL array dimensioned (NBP)	Total carbon load to cell from External Load File 2.	kg day^{-1}
S3FLXCB	A REAL array dimensioned (NBP)	Total carbon load to cell from External Load File 3.	kg day^{-1}
DLSEDKNB	A REAL array dimensioned (NSBP)	Total nitrogen source or sink in sediment cell due to kinetics. The sole term is loss due to denitrification.	kg day^{-1}
BURIALFLXNB	A REAL array dimensioned (NSBP)	Burial of total nitrogen from sediment cell to deep sediments.	kg day^{-1}
BURIALFLXPB	A REAL array dimensioned (NSBP)	Burial of total phosphorus from sediment cell to deep sediments.	kg day^{-1}

DLSEDKCB	A REAL array dimensioned (NSBP)	Total carbon source or sink in sediment cell due to kinetics. The sole term is loss due to diagenesis.	kg day^{-1}
BURIALFLXCB	A REAL array dimensioned (NSBP)	Burial of organic carbon from sediment cell to deep sediments.	kg day^{-1}

Additional Information

The array SBN contains the cell numbers of surface cells in the order they are entered in the Geometry File. Figure 1 shows an elevation of a thirty-box grid (10 cells long by 3 cells deep). For this grid, the contents of array SBN are:

SBN(1) = 1, SBN(2) = 2, ... SBN(10) = 10

Since the surface cells were entered in numerical order, the array SBN is redundant in this case.

The array BBN contains the cell numbers of bottom cells in the order they are entered in the Geometry File. For the grid in Figure 1, the contents of array BBN are:

BBN(1) = 21, BBN(2) = 22, ... BBN(10) = 30

The array BBN is useful as a reference to link conditions in the sediments to conditions in overlying water-column cells.

Mass balances can be listed relative to water-column or sediment cells. For sources such as atmospheric loads and sinks such as burial, the reference to a water-column or sediment cell is obvious as is the sign convention. For mass balances that quantify transfers between water and sediments, the reference and sign convention are not obvious. These fluxes include BENFLXPNB, BENFLXDNB, BENFLXPPB, BENFLXDPB, and BENFLXPCB. For these fluxes, the array element refers to a sediment cell. The sign convention is that **positive fluxes are sources to the water column**. For example, the settling of particulate carbon from water-column cell 10 to sediment cell 1 is BENFLXPCB(1). This variable is output from the model as a negative quantity since it is a loss from the water column.

The Kinetics Flux File

The Kinetics Flux File is a complement to the Transportation Flux File and the Mass-Balance File. The Kinetics Flux File contains the rates of substance transformations in the water column due to kinetics processes. Information to aid in interpretation of kinetics fluxes (including temperature, dissolved oxygen concentration, and algal growth rates) is also provided.

Kinetics fluxes are output when "KFLC = ON" is specified in the Kinetics Flux Output Control card group in the Control File. Kinetics fluxes are averaged over user-specified intervals. The averaging interval is also specified in the Kinetics Flux Output Control card group.

Header information is written to the Kinetics Flux File once when it is opened. The WRITE statement is:

```
WRITE (KFL) TITLE, NB, NSB, SBN, BBN, V1,
     .  SFA, SAV_CALC, BALGAE_CALC
```

Subsequent information is written to the Kinetics Flux File repeatedly at intervals specified in the Kinetics Flux Output Control card group. The WRITE statements are:

```
WRITE(KFL) JDAY

WRITE(KFL) A_T,      AP1,      ABM1,     APR1,
     .             AP2,      ABM2,     APR2,     AP3,
     .             ABM3,     APR3

WRITE(KFL) AALGDOC,  AALGPOC,  ADENIT,   AMNLDOC,
     .     AHDRLPOC, AHDRRPOC

WRITE(KFL) AALGNH4,  AALGNO3,  AALGDON,  AALGPON,
     .     ANT,      ADENNO3,  AMNLDON,  AHDRLPON,
     .               AHDRRPON

WRITE(KFL) AALGPO4,  AALGDOP,  AALGPOP,  AMNLDOP,
     .               AHDRLPOP, AHDRRPOP

WRITE(KFL) APSD,     ASAP,     AALGUP,   AALGRES

WRITE(KFL) ADO,      ADORALG,  ADOPR,    ADCOD,
     .               ADDOC,    ANITRIF

WRITE(KFL) ARSZ,  ARLZ,   ABMSZ,   ABMLZ,
     .     AMSZ,   AMLZ,   APRSZLZ, AGSZ,  AGLZ,   ADOCSZ,
     .     ALPOCSZ,ARPOCSZ,ADOCLZ,  ALPOCLZ,       ARPOCLZ,
     .     ANH4SZ, ADONSZ, ALPONSZ, ARPONSZ,       ANH4LZ,
     .     ADONLZ, ALPONLZ,ARPONLZ, APO4SZ,ADOPSZ, ALPOPSZ,
     .     ARPOPSZ,APO4LZ, ADOPLZ,  ALPOPLZ,       ARPOPLZ,
     .     APRSZ,  APRLZ

WRITE(KFL) AB1SZ,  AB2SZ,  AB3SZ,   AB1LZ, AB2LZ,  AB3LZ,
     .     ADOSZ,  ADOLZ,  ASASZ,   ASUSZ, ASALZ,  ASULZ

IF (SAV_CALC) THEN

   WRITE(KFL) APSH,   ABMSH,    ABMRT,    ASLSH,
     .        APEP,   ABMEP,    APREP

   WRITE(KFL) ADOCSAV,  ALPOCSAV, ARPOCSAV, ADOCEPI,
     .        ALPOCEPI, ARPOCEPI, ASEDCSAV, ANH4SAVW,
```

```
     .         ANO3SAVW, ADONSAVW, ALPONSAVW,ARPONSAVW,
     .         ANH4EPI,  ANO3EPI,  ADONEPI,  ALPONEPI,
     .         ARPONEPI, ASEDNSAV, ASEDNH4SAV,APO4SAVW,
     .         ADOPSAVW, ALPOPSAVW,ARPOPSAVW,APO4EPI,
     .         ADOPEPI,  ALPOPEPI, ARPOPEPI, ASEDPSAV,
     .         ASEDPO4SAV,ADOSAV,  ADOEPI,   ASEDDOSAV

END IF

IF (BALGAE_CALC) WRITE(KFL)
     .  ABMB,      APB,       APRB,      ABADOC,
     .  ABAPOC,    ABANH4,    ABANO3,    ABAPON,
     .  ABAPO4,    ABAPOP,    ABADO
```

Variables in the WRITE statements are summarized in Table 7.

Table 7
Variables Written to Kinetics Flux File

Variable	Type	Definition	Units
TITLE	An array with six elements. Each element is CHARACTER*72.	Six title lines from the head of the control file.	
NB	INTEGER	Number of cells in model grid	
NSB	INTEGER	Number of surface cells in grid	
SBN	An INTEGER array dimensioned (NSBP). NSBP = maximum number of surface cells. NSBP is assigned in INCLUDE file.	An array of surface cell numbers.	
BBN	An INTEGER array dimensioned (NSBP)	An array of bottom cell numbers.	
V1	A REAL*8 array dimensioned (0:NBP). NBP=maximum number of cells assigned in the INCLUDE file.	Volume of model cell	m^3
SFA	A REAL array dimensioned (NSBP). NSBP=maximum number of surface cells assigned in the INCLUDE file.	Surface area of model cell	m^2

SAV_CALC	Logical	.TRUE. if SAV submodel is ON. .FALSE. otherwise.	
BALGAE_CALC	Logical	.TRUE. if benthic algae are calculated. .FALSE. otherwise.	
JDAY	REAL	Julian day elapsed since beginning of run	day
A_T	A REAL array dimensioned (NBP)	Temperature	C^o
AP1	A REAL array dimensioned (NBP)	Algal group 1 specific growth rate	day^{-1}
ABM1	A REAL array dimensioned (NBP)	Algal group 1 specific respiration rate	day^{-1}
APR1	A REAL array dimensioned (NBP)	Rate of predation on algal group 1	gm C m^{-3} day^{-1}
AP2	A REAL array dimensioned (NBP)	Algal group 2 specific growth rate	day^{-1}
ABM2	A REAL array dimensioned (NBP)	Algal group 2 specific respiration rate	day^{-1}
APR2	A REAL array dimensioned (NBP)	Rate of predation on algal group 2	gm C m^{-3} day^{-1}
AP3	A REAL array dimensioned (NBP)	Algal group 3 specific growth rate	day^{-1}
ABM3	A REAL array dimensioned (NBP)	Algal group 3 specific respiration rate	day^{-1}
APR3	A REAL array dimensioned (NBP)	Rate of predation on algal group 3	gm C m^{-3} day^{-1}
AALGDOC	A REAL array dimensioned (NBP)	Dissolved organic carbon production by all algae	gm C m^{-3} day^{-1}
AALGPOC	A REAL array dimensioned (NBP)	Particulate organic carbon production by all algae	gm C m^{-3} day^{-1}
ADENIT	A REAL array dimensioned (NBP)	Loss of dissolved organic carbon by denitrification	gm C m^{-3} day^{-1}
AMNLDOC	A REAL array dimensioned (NBP)	Respiration of dissolved organic carbon	gm C m^{-3} day^{-1}
AHDRLPOC	A REAL array dimensioned (NBP)	Hydrolysis of labile particulate organic carbon	gm C m^{-3} day^{-1}
AHDRRPOC	A REAL array dimensioned (NBP)	Hydrolysis of refractory particulate organic carbon	gm C m^{-3} day^{-1}
AALGNH4	A REAL array dimensioned (NBP)	Algal uptake /production of ammonium. See explanation below.	gm N m^{-3} day^{-1}

AALGNO3	A REAL array dimensioned (NBP)	Algal uptake of nitrate	gm N m^{-3} day^{-1}
AALGDON	A REAL array dimensioned (NBP)	Algal production of dissolved organic nitrogen	gm N m^{-3} day^{-1}
AALGPON	A REAL array dimensioned (NBP)	Algal production of particulate organic nitrogen	gm N m^{-3} day^{-1}
ANT	A REAL array dimensioned (NBP)	Loss of ammonium through nitrification	gm N m^{-3} day^{-1}
ADENNO3	A REAL array dimensioned (NBP)	Loss of nitrate through denitrification	gm N m^{-3} day^{-1}
AMNLDON	A REAL array dimensioned (NBP)	Mineralization of dissolved organic nitrogen	gm N m^{-3} day^{-1}
AHDRLPON	A REAL array dimensioned (NBP)	Hydrolysis of labile particulate organic nitrogen	gm N m^{-3} day^{-1}
AHDRRPON	A REAL array dimensioned (NBP)	Hydrolysis of refractory particulate organic nitrogen	gm N m^{-3} day^{-1}
AALGPO4	A REAL array dimensioned (NBP)	Net loss of total phosphate due to algal activity. See explanation below.	gm P m^{-3} day^{-1}
AALGDOP	A REAL array dimensioned (NBP)	Algal production of dissolved organic phosphorus	gm P m^{-3} day^{-1}
AALGPOP	A REAL array dimensioned (NBP)	Algal production of particulate organic phosphorus	gm P m^{-3} day^{-1}
AMNLDOP	A REAL array dimensioned (NBP)	Mineralization of dissolved organic phosphorus	gm P m^{-3} day^{-1}
AHDRLPOP	A REAL array dimensioned (NBP)	Hydrolysis of labile particulate organic phosphorus	gm P m^{-3} day^{-1}
AHDRRPOP	A REAL array dimensioned (NBP)	Hydrolysis of refractory particulate organic phosphorus	gm P m^{-3} day^{-1}
APSD	A REAL array dimensioned (NBP)	Dissolution of particulate to dissolved silica	gm Si m^{-3} day^{-1}
ASAP	A REAL array dimensioned (NBP)	Production of dissolved silica through predation	gm Si m^{-3} day^{-1}
AALGUP	A REAL array dimensioned (NBP)	Silica uptake by algae	gm Si m^{-3} day^{-1}
AALGRES	A REAL array dimensioned (NBP)	Dissolved silica release by algal respiration	gm Si m^{-3} day^{-1}

ADO	A REAL array dimensioned (NBP)	Dissolved oxygen concentration	gm m^{-3}
ADORALG	A REAL array dimensioned (NBP)	Net algal oxygen production /consumption. See explanation below.	gm O_2 m^{-3} day^{-1}
ADOPR	A REAL array dimensioned (NBP)	Direct oxygen uptake by predators	gm O_2 m^{-3} day^{-1}
ADCOD	A REAL array dimensioned (NBP)	Oxygen loss through chemical oxygen demand	gm O_2 m^{-3} day^{-1}
ADDOC	A REAL array dimensioned (NBP)	Oxygen loss through respiration of dissolved organic carbon	gm O_2 m^{-3} day^{-1}
ANITRIF	A REAL array dimensioned (NBP)	Oxygen loss through nitrification	gm O_2 m^{-3} day^{-1}
ARSZ	A REAL array dimensioned (NBP)	Microzooplankton ration	g prey C g^{-1} predator C d^{-1}
ARLZ	A REAL array dimensioned (NBP)	Mesoozooplankton ration	g prey C g^{-1} predator C d^{-1}
ABMSZ	A REAL array dimensioned (NBP)	Microzooplankton specific respiration rate	d^{-1}
ABMLZ	A REAL array dimensioned (NBP)	Mesozooplankton specific respiration rate	d^{-1}
AMSZ	A REAL array dimensioned (NBP)	Microzooplankton mortality due to low DO	d^{-1}
AMLZ	A REAL array dimensioned (NBP)	Mesozooplankton mortality due to low DO	d^{-1}
APRSZLZ	A REAL array dimensioned (NBP)	Predation on microzooplankton by mesozooplankton	g C m^{-3} d^{-1}
AGSZ	A REAL array dimensioned (NBP)	Specific growth rate for microzooplankton	d^{-1}
AGLZ	A REAL array dimensioned (NBP)	Specific growth rate for mesozooplankton	d^{-1}
ADOCSZ	A REAL array dimensioned (NBP)	DOC production by microzooplankton	gm C m^{-3} day^{-1}
ALPOCSZ	A REAL array dimensioned (NBP)	LPOC production by microzooplankton	gm C m^{-3} day^{-1}
ARPOCSZ	A REAL array dimensioned (NBP)	RPOC production by microzooplankton	gm C m^{-3} day^{-1}
ADOCLZ	A REAL array dimensioned (NBP)	DOC production by mesozooplankton	gm C m^{-3} day^{-1}

ALPOCLZ	A REAL array dimensioned (NBP)	LPOC production by mesozooplankton	gm C m^{-3} day^{-1}
ARPOCLZ	A REAL array dimensioned (NBP)	RPOC production by mesozooplankton	gm C m^{-3} day^{-1}
ANH4SZ	A REAL array dimensioned (NBP)	Ammonium production by microzooplankton	gm N m^{-3} day^{-1}
ADONSZ	A REAL array dimensioned (NBP)	DON production by microzooplankton	gm N m^{-3} day^{-1}
ALPONSZ	A REAL array dimensioned (NBP)	LPON production by microzooplankton	gm N m^{-3} day^{-1}
ARPONSZ	A REAL array dimensioned (NBP)	RPON production by microzooplankton	gm N m^{-3} day^{-1}
ANH4LZ	A REAL array dimensioned (NBP)	Ammonium production by mesozooplankton	gm N m^{-3} day^{-1}
ADONLZ	A REAL array dimensioned (NBP)	DON production by mesozooplankton	gm N m^{-3} day^{-1}
ALPONLZ	A REAL array dimensioned (NBP)	LPON production by mesozooplankton	gm N m^{-3} day^{-1}
ARPONLZ	A REAL array dimensioned (NBP)	RPON production by mesozooplankton	gm N m^{-3} day^{-1}
APO4SZ	A REAL array dimensioned (NBP)	Phosphate production by microzooplankton	gm P m^{-3} day^{-1}
ADOPSZ	A REAL array dimensioned (NBP)	DOP production by microzooplankton	gm P m^{-3} day^{-1}
ALPOPSZ	A REAL array dimensioned (NBP)	LPOP production by microzooplankton	gm P m^{-3} day^{-1}
ARPOPSZ	A REAL array dimensioned (NBP)	RPOP production by microzooplankton	gm P m^{-3} day^{-1}
APO4LZ	A REAL array dimensioned (NBP)	Phosphate production by mesozooplankton	gm P m^{-3} day^{-1}
ADOPLZ	A REAL array dimensioned (NBP)	DOP production by mesozooplankton	gm P m^{-3} day^{-1}
ALPOPLZ	A REAL array dimensioned (NBP)	LPOP production by mesozooplankton	gm P m^{-3} day^{-1}
ARPOPLZ	A REAL array dimensioned (NBP)	RPOP production by mesozooplankton	gm P m^{-3} day^{-1}
APRSZ	A REAL array dimensioned (NBP)	Predation on microzooplankton	gm C m^{-3} day^{-1}
APRLZ	A REAL array dimensioned (NBP)	Predation on mesozooplankton	gm C m^{-3} day^{-1}

AB1SZ	A REAL array dimensioned (NBP)	Microzooplankton consumption of algal group 1	gm C m^{-3} day^{-1}
AB2SZ	A REAL array dimensioned (NBP)	Microzooplankton consumption of algal group 2	gm C m^{-3} day^{-1}
AB3SZ	A REAL array dimensioned (NBP)	Microzooplankton consumption of algal group 3	gm C m^{-3} day^{-1}
AB1LZ	A REAL array dimensioned (NBP)	Mesozooplankton consumption of algal group 1	gm C m^{-3} day^{-1}
AB2LZ	A REAL array dimensioned (NBP)	Mesozooplankton consumption of algal group 2	gm C m^{-3} day^{-1}
AB3LZ	A REAL array dimensioned (NBP)	Mesozooplankton consumption of algal group 3	gm C m^{-3} day^{-1}
ADOSZ	A REAL array dimensioned (NBP)	Microzooplankton consumption of dissolved oxygen	gm DO m^{-3} day^{-1}
ADOLZ	A REAL array dimensioned (NBP)	Mesozooplankton consumption of dissolved oxygen	gm DO m^{-3} day^{-1}
ASASZ	A REAL array dimensioned (NBP)	Microzooplankton production of dissolved silica	gm Si m^{-3} day^{-1}
ASUSZ	A REAL array dimensioned (NBP)	Microzooplankton production of particulate biogenic silica	gm Si m^{-3} day^{-1}
ASALZ	A REAL array dimensioned (NBP)	Mesozooplankton production of dissolved silica	gm Si m^{-3} day^{-1}
ASULZ	A REAL array dimensioned (NBP)	Mesozooplankton production of particulate biogenic silica	gm Si m^{-3} day^{-1}
APSH	A REAL array dimensioned (NSBP)	SAV shoot specific growth rate	d^{-1}
ABMSH	A REAL array dimensioned (NSBP)	SAV shoot specific respiration rate	d^{-1}
ABMRT	A REAL array dimensioned (NSBP)	SAV root specific respiration rate	d^{-1}
ASLSH	A REAL array dimensioned (NSBP)	SAV shoot specific sloughing rate	d^{-1}
APEP	A REAL array dimensioned (NSBP)	Epiphyte specific growth rate	d^{-1}
ABMEP	A REAL array dimensioned (NSBP)	Epiphyte specific respiration rate	d^{-1}
APREP	A REAL array dimensioned (NSBP)	Specific predation on epiphytes	d^{-1}
ADOCSAV	A REAL array dimensioned (NSBP)	SAV DOC release to water column	gm C m^{-2} day^{-1}

ALPOCSAV	A REAL array dimensioned (NSBP)	SAV LPOC release to water column	gm C m^{-2} day^{-1}
ARPOCSAV	A REAL array dimensioned (NSBP)	SAV RPOC release to water column	gm C m^{-2} day^{-1}
ADOCEPI	A REAL array dimensioned (NSBP)	Epiphyte DOC release to water column	gm C m^{-2} day^{-1}
ALPOCEPI	A REAL array dimensioned (NSBP)	Epiphyte LPOC release to water column	gm C m^{-2} day^{-1}
ARPOCEPI	A REAL array dimensioned (NSBP)	Epiphyte RPOC release to water column	gm C m^{-2} day^{-1}
ASEDCSAV	A REAL array dimensioned (NSBP)	SAV organic carbon release to sediments	gm C m^{-2} day^{-1}
ANH4SAVW	A REAL array dimensioned (NSBP)	SAV ammonium exchange with water column	gm N m^{-2} day^{-1}
ANO3SAVW	A REAL array dimensioned (NSBP)	SAV nitrate uptake from water column	gm N m^{-2} day^{-1}
ADONSAVW	A REAL array dimensioned (NSBP)	SAV DON release to water column	gm N m^{-2} day^{-1}
ALPONSAVW	A REAL array dimensioned (NSBP)	SAV LPON release to water column	gm N m^{-2} day^{-1}
ARPONSAVW	A REAL array dimensioned (NSBP)	SAV RPON release to water column	gm N m^{-2} day^{-1}
ANH4EPI	A REAL array dimensioned (NSBP)	Epiphyte ammonium exchange with water column	gm N m^{-2} day^{-1}
ANO3EPI	A REAL array dimensioned (NSBP)	Epiphyte nitrate uptake from water column	gm N m^{-2} day^{-1}
ADONEPI	A REAL array dimensioned (NSBP)	Epiphyte DON release to water column	gm N m^{-2} day^{-1}
ALPONEPI	A REAL array dimensioned (NSBP)	Epiphyte LPON release to water column	gm N m^{-2} day^{-1}
ARPONEPI	A REAL array dimensioned (NSBP)	Epiphyte RPON release to water column	gm N m^{-2} day^{-1}
ASEDNSAV	A REAL array dimensioned (NSBP)	SAV organic nitrogen release to sediments	gm N m^{-2} day^{-1}
ASEDNH4SAV	A REAL array dimensioned (NSBP)	SAV ammonium uptake from sediments	gm N m^{-2} day^{-1}
APO4SAVW	A REAL array dimensioned (NSBP)	SAV phosphate exchange with water column	gm P m^{-2} day^{-1}
ADOPSAVW	A REAL array dimensioned (NSBP)	SAV DOP release to water column	gm P m^{-2} day^{-1}

ALPOPSAVW	A REAL array dimensioned (NSBP)	SAV LPOP release to water column	gm P m^{-2} day^{-1}
ARPOPSAVW	A REAL array dimensioned (NSBP)	SAV RPOP release to water column	gm P m^{-2} day^{-1}
APO4EPI	A REAL array dimensioned (NSBP)	Epiphyte phosphate exchange with water column	gm P m^{-2} day^{-1}
ADOPEPI	A REAL array dimensioned (NSBP)	Epiphyte DOP release to water column	gm P m^{-2} day^{-1}
ALPOPEPI	A REAL array dimensioned (NSBP)	Epiphyte LPOP release to water column	gm P m^{-2} day^{-1}
ARPOPEPI	A REAL array dimensioned (NSBP)	Epiphyte RPOP release to water column	gm P m^{-2} day^{-1}
ASEDPSAV	A REAL array dimensioned (NSBP)	SAV organic phosphorus release to sediments	gm P m^{-2} day^{-1}
ASEDPO4SAV	A REAL array dimensioned (NSBP)	SAV phosphate uptake from sediments	gm P m^{-2} day^{-1}
ADOSAV	A REAL array dimensioned (NSBP)	SAV dissolved oxygen exchange with water column	gm O_2 m^{-2} day^{-1}
ADOEPI	A REAL array dimensioned (NSBP)	Epiphyte dissolved oxygen exchange with water column	gm O_2 m^{-2} day^{-1}
ASEDDOSAV	A REAL array dimensioned (NSBP)	Dissolved oxygen transferred from SAV shoots to roots	gm O_2 m^{-2} day^{-1}
ABMB	A REAL array dimensioned (NSBP)	Benthic algae specific respiration rate	day^{-1}
APB	A REAL array dimensioned (NSBP)	Benthic algae specific growth rate	day^{-1}
APRB	A REAL array dimensioned (NSBP)	Benthic algae specific predation rate	day^{-1}
ABADOC	A REAL array dimensioned (NSBP)	Benthic algae DOC release rate	gm C m^{-2} day^{-1}
ABAPOC	A REAL array dimensioned (NSBP)	POC released to sediments by benthic algae	gm C m^{-2} day^{-1}
ABANH4	A REAL array dimensioned (NSBP)	Ammonium uptake/release by benthic algae	gm N m^{-2} day^{-1}
ABANO3	A REAL array dimensioned (NSBP)	Nitrate uptake by benthic algae	gm N m^{-2} day^{-1}
ABAPON	A REAL array dimensioned (NSBP)	PON released to sediments by benthic algae	gm N m^{-2} day^{-1}
ABAPO4	A REAL array dimensioned (NSBP)	Phosphate uptake/release by benthic algae	gm P m^{-2} day^{-1}

ABAPOP	A REAL array dimensioned (NSBP)	POP released to sediments by benthic algae	gm P m^{-2} day^{-1}
ABADO	A REAL array dimensioned (NSBP)	Dissolved oxygen uptake/release by benthic algae	gm O_2 m^{-2} day^{-1}

Additional Information

Algae take up ammonium during growth (production) and release ammonium through respiration and the actions of predation. The variable AALGNH4 is the sum of all algal processes affecting ammonium. If the quantity is positive, ammonium release through respiration and predation exceeds uptake through growth. If the quantity is negative, uptake due to growth exceeds losses through respiration and predation. Exchanges of phosphate and dissolved oxygen are treated similarly.

The Oxygen Volume Output File

The Oxygen Volume Output File contains statistics that quantify the volume-time integral of dissolved oxygen within a specified range. The statistics are termed "dissolved-oxygen volume days". Dissolved-oxygen volume days are a useful statistic for comparison of dissolved-oxygen improvements during model scenario runs.

The dissolved-oxygen volume days statistic is defined:

$$DOVD_{i,j} = V_i \int_{T_1}^{T_2} f(j)\,dt \qquad \textbf{(1)}$$

$DOVD_{i,j}$ = dissolved oxygen volume days in cell i within oxygen interval j (m^3 days)
V_i = volume of cell i (m^3)
T_1 = beginning of integration interval (day)
T_2 = end of integration interval (day)

The function f(j) has two potential values:

$$f(j) = 1 \quad \text{when } LLIM_j \le DO_i < ULIM_j \qquad \textbf{(2)}$$

or

$$f(j) = 0 \quad \text{otherwise} \qquad \textbf{(3)}$$

DO_i = dissolved oxygen concentration in cell i (gm O_2 m^{-3})
$LLIM_j$ = lower limit of dissolved oxygen interval j (gm O_2 m^{-3})
$ULIM_j$ = upper limit of dissolved oxygen interval j (gm O_2 m^{-3})

The Oxygen Volume Output File is produced when "OPLC = ON" is specified in the Oxygen Plot Output Control card group in the Control File. The dissolved-oxygen intervals and integration periods are specified in the same card group.

Header information is written to the Oxygen Volume Output File once when it is opened. The WRITE statement is:

```
WRITE (OPL) TITLE,NB,NOINT,OINT,V1
```

Subsequent information is written to the Oxygen Volume Output File repeatedly at intervals specified in the Oxygen Plot Output Control card group. The WRITE statement is:

```
WRITE (OPL) JDAY,DOVDAYS
```

Variables in the WRITE statements are summarized in Table 8.

Table 8
Variables Written to Oxygen Volume Output File

Variable	Type	Definition	Units
TITLE	An array with six elements. Each element is CHARACTER*72.	Six title lines from the head of the Control File	
NB	INTEGER	Number of cells in model grid	
NOINT	INTEGER	Number of dissolved oxygen concentration intervals	
OINT	A REAL array dimensioned (NOIP). NOIP=maximum number of oxygen intervals assigned in the INCLUDE file.	Dissolved oxygen concentration intervals	gm m^{-3}
V1	A REAL*8 array dimensioned (0:NBP). NBP=maximum number of cells assigned in the INCLUDE file.	Volume of model cell	m^3
JDAY	REAL	Julian day elapsed since beginning of run	day
DOVDAYS	A REAL array dimensioned (NBP,NOIP)	Dissolved-oxygen volume days. See explanation below.	m^3 day

Additional Information

The first subscript of the DOVDAYS array indicates cell number. The

second subscript indicates oxygen interval. For example, DOVDAYS(10,2) is the dissolved-oxygen volume days in cell 10 within oxygen interval 2. Note that the number of computed intervals is always one fewer than the number of intervals specified as NOINT. Decrement by one occurs because both upper and lower limits to oxygen intervals must be specified in array OINT.

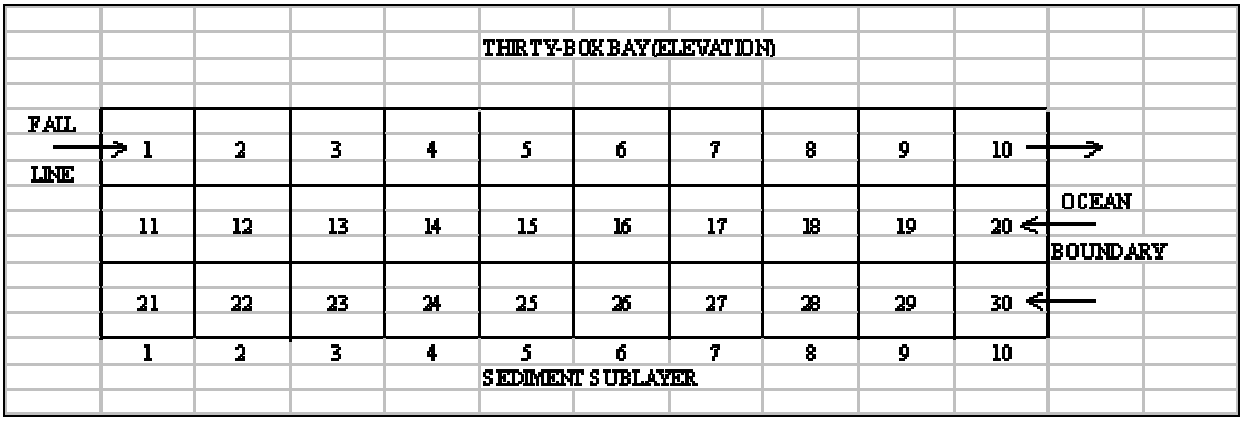

Figure 1. Elevation of thirty-box grid