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Waterways Experiment
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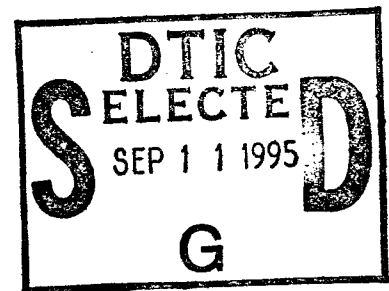
CE-QUAL-W2: A Two-Dimensional, Laterally Averaged, Hydrodynamic and Water Quality Model, Version 2.0

User Manual

by Thomas M. Cole, WES

Edward M. Buchak, J. E. Edinger Associates, Inc.

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CE-QUAL-W2: A Two-Dimensional, Laterally Averaged, Hydrodynamic and Water Quality Model, Version 2.0

User Manual

by Thomas M. Cole

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Final report

Prepared for   U.S. Army Corps of Engineers
   Washington, DC 20314-1000

**US Army Corps
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STRUCTURES
LABORATORY

SCALE

800   0   800 m

AREA OF RESERVATION = 2.7 sq km

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Preface

This manual documents the two-dimensional, laterally averaged, hydrody-namic and water quality model CE-QUAL-W2. This manual was prepared in the Environmental Laboratory (EL), U.S. Army Engineer Waterways Experi-ment Station (WES), Vicksburg, MS. Funding for Version 2.0 of the manual was provided by Headquarters, U.S. Army Corps of Engineers (HQUSACE), under the Numerical Model Maintenance Program.

The Principal Investigator for Version 2.0 of CE-QUAL-W2 and the User Manual was Mr. Thomas M. Cole of the Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Effects Division (EPED), EL. This report was prepared by Mr. Cole and Mr. Edward M. Buchak, J. E. Edinger Associates, Inc., Wayne, PA, under the direct supervision of Dr. Mark S. Dortch, Chief, WQCMB, and under the general supervision of Mr. Donald L. Robey, Chief, EPED, and Dr. John W. Keeley, Director, EL. Technical reviews by Dr. Dortch, Dr. Billy Johnson, and Mr. Ross Hall are gratefully acknowledged.

At the time of publication of this manual, Director of WES was Dr. Robert W. Whalin. Commander of WES was COL Bruce K. Howard, EN.

This report shoud be cited as follows:

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Model Package

All files on the CE-QUAL-W2 distribution disk are archived in self-extracting files. To install CE-QUAL-W2 from the distribution disk to a hard disk, copy over the compressed file "W2.EXE" on a PC's hard disk. To decompress the files, enter "W2" at the DOS prompt. The "read_me.1st" file contains an explanation of the subdirectory structure and files which will be setup on the PC.

Several example applications are included in the subdirectory "EXAMPLES". The Degray application is a reservoir with a single branch and a complete water quality application. The J. Strom Thurmond (JST) application modeled 10km of JST reservoir below Richard B. Russell Dam on the Savannah River between Georgia and South Carolina. A downstream boundary head was applied since the entire reservoir was not modeled. Three branches were included and withdrawals were used to simulate pump-storage. Only DO and temperature were modeled. DO was treated as conservative except for atmospheric rearation since the modeling period was only 2 days.

The Raritan river application modeled an east coast estuary for temperature, salinity, velocities, and water surface elevations. The Cheatham Reservoir application modeled a stretch of the Cumberland River near Nashville, TN for water quality and included the effects of BOD loadings on dissolved oxygen.

Programs

The following FORTRAN files are located in the SOURCE subdirectory:

W2.FOR   - CE-QUAL-W2 generic version
W2_LAH.FOR   - CE-QUAL-W2 Lahey FORTRAN version
W2_FTN.FOR   - CE-QUAL-W2 FTN77 FORTRAN version
W2_UNIX.FOR - CE-QUAL-W2 unix workstation version
PRE.FOR   - Generic preprocessor
PRE_LAH.FOR - Lahey FORTRAN preprocessor
PRE_OTG.FOR - FTN77 FORTRAN preprocessor
W2.INC   - Include file containing the user modifiable code necessary
                      to set up the model for a particular application

Input Files

The following input files come with each application:

W2_CON.NPT - Control file for each application
BTH.NPT   - Bathymetry file
MET.NPT   - Meteorological file

A subset of the following input files comes with each application:

QIN_BR1.NPT - Inflows
TIN_BR1.NPT - Inflow temperatures
CIN_BR1.NPT - Inflow constituent concentrations
QTR_TR1.NPT - Tributary inflows
TTR_TR1.NPT - Tributary inflow temperatures
CTR_TR1.NPT - Tributary inflow constituent concentrations
EUH_BR1.NPT - Upstream head elevations
TUH_BR1.NPT - Upstream head boundary temperatures
CUH_BR1.NPT - Upstream head boundary constituent concentrations
EDH_BR1.NPT - Downstream head elevations
TDH_BR1.NPT - Downstream head boundary temperatures
CDH_BR1.NPT - Downstream head boundary constituent concentrations
QOT_BR1.NPT - Outflows
QWD_BR1.NPT - Withdrawals
VPR.NPT   - Vertical profile at dam for specifying initial conditions
LPR.NPT   - Longitudinal and vertical profiles specifying initial conditions for each cell

If more than one branch or tributary is modeled, then corresponding files using
"BR2", "BR3", etc. (or "TR2, "TR3", etc.) in the filename will also be included.

Output Files

The following output files come with each application:

SNP.SAV - Snapshot output file in ASCII with interpretation of FORTRAN carriage control characters
PRE.SAV - Preprocessor output file

The snapshot files are from a short run of the application. Use these files to ensure you obtain the same answers. These files are setup to be printed on a LaserJet IV compatible printer. The FORTRAN compiler used to make these test runs was Lahey F77L3-EM/32 V5.10.

Computer Requirements

Hardware. The minimum configuration is an 80386 PC equipped with a math coprocessor. A minimum of four megabytes of memory is needed unless the user has an operating system or extender that uses virtual memory. A hard disk with a minimum available space of 25 Mb is also required.

Software. For an 80386 or greater PC operating under DOS, the user must have a 32 bit FORTRAN compiler with a DOS extender that will allow the model to utilize protected mode. The model has been tested on the following 32-bit PC compilers:

1. Lahey
2. FTN77
3. Microsoft PowerStation

If the user has either a Unix, OS/2, or Windows NT operating system, then a FORTRAN compiler that is compatible with the operating system is required. These operating systems remove the 640K memory limit and thus do not require an extender. The model has also been tested on Silicon Graphics, DEC Alpha, and Hewlett-Packard workstations, VAX minicomputers, and Cray supercomputers.

1 Introduction

Model Overview

CE-QUAL-W2 is a two-dimensional, longitudinal/vertical, hydrodynamic and water quality model. Because the model assumes lateral homogeneity, it is best suited for relatively long and narrow waterbodies exhibiting longitudinal and vertical water quality gradients. The model has been applied to rivers, lakes, reservoirs, and estuaries.

The application of CE-QUAL-W2 requires knowledge in the following areas:

1. Hydrodynamics
2. Aquatic biology
3. Aquatic chemistry
4. Numerical methods
5. Computers and FORTRAN coding
6. Statistics
7. Data assembly and reconstruction

Water quality modeling is in many ways an art requiring not only knowledge in these areas but experience in their integration. *A word of caution to the first time user* - model application is a complicated and time consuming task.

Model Background

Version 1.0. CE-QUAL-W2 has been under continuous development since 1975. The original model was known as LARM (*L*aterally *A*veraged *R*eservoir *M*odel) developed by Edinger and Buchak (1975). The first LARM application was on a reservoir with no branches. Subsequent modifications to allow for multiple branches and estuarine boundary conditions resulted in the code known as GLVHT (*G*eneralized *L*ongitudinal-*V*ertical *H*ydrodynamics and *T*ransport Model). Addition of the water quality algorithms by the Water Quality Modeling Group at the US Army Engineer Waterways Experiment Station (WES) resulted in CE-QUAL-W2 Version 1.0 (Environmental and Hydraulic Laboratories, 1986).

Version 2.0. Version 2.0 is a result of major modifications to the code to improve the mathematical description of the prototype and increase computa-

tional accuracy and efficiency. Numerous new capabilities have been included in Version 2.0. These are:

  a. an algorithm that calculates the maximum allowable timestep and adjusts the timestep to ensure hydrodynamic stability requirements are not violated (autostepping)
  b. a selective withdrawal algorithm that calculates a withdrawal zone based on outflow, outlet geometry, and upstream density gradients
  c. a higher-order transport scheme (QUICKEST) that reduces numerical diffusion (Leonard, 1979)
  d. time-weighted vertical advection and fully implicit vertical diffusion
  e. step function or linear interpolation of inputs
  f. improved ice-cover algorithm
  g. internal calculation of equilibrium temperatures and coefficients of surface heat exchange or a term-by-term accounting of surface heat exchange
  h. variable layer heights and segment lengths
  i. surface layer extending through multiple layers
  j. generalized time-varying data input subroutine with input data accepted at any frequency
  k. volume and mass balances to machine accuracy
  l. sediment/water heat exchange

Considerable effort has also been made to make the model easier to use. The input and output data have been reformatted and the user manual has been rewritten with this goal in mind.

Manual

Organization. The manual has been rewritten so the first time user is not initially hampered with the model's burdensome details. It is intended to familiarize the user to the overall steps necessary in applying the model. It is organized into three chapters and four appendices. Chapter 1 consists of an introduction to the model and the user manual. Chapter 2 describes the model's major capabilities and limitations. Chapter 3 provides an overview of the steps involved in applying the model including data preparation and model application.

The appendices provide the user with the information necessary to understand the model details. Appendix A describes the theoretical, numerical, and computational basis for the hydrodynamic portion of the model. Appendix B describes the theoretical and computational basis for the water quality portion of

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the model. Appendix C describes the preparation of input files. Appendix D describes the algorithms used in the code. References include a partial bibliography of CE-QUAL-W2 applications. An index is also included.

A major goal in rewriting the user manual was to allow easy access to the tremendous amount of information in the manual. The following concepts have been used to accomplish this goal:

1. Page headers are used to allow the user to easily find major areas in the manual.
2. Where applicable, paragraphs contain descriptive headings for easy reference.
3. Page references are used when related information is contained elsewhere.
4. An index is located at the end of the manual.

Conventions. References to FORTRAN variables in the manual are made in English and are followed by their FORTRAN name enclosed by brackets (eg., surface layer [KT]). The user need not first memorize the variable names to comprehend the manual. Potential problem areas in applying the model are emphasized with ***bold italic*** type.

2 Capabilities and Limitations

Capabilities

Hydrodynamic. The model predicts water surface elevations, velocities, and temperatures. Temperature is included in the hydrodynamic calculations because of its effect on water density.

Water quality. The water quality algorithms incorporate 21 constituents in addition to temperature including nutrient/phytoplankton/dissolved oxygen (DO) interactions during anoxic conditions. Any combination of constituents can be simulated. The effects of salinity or total dissolved solids/salinity on density and thus hydrodynamics are included only if they are simulated in the water quality module. The water quality algorithm is modular allowing constituents to be easily added as additional subroutines.

Long term simulations. The water surface elevation is solved implicitly which eliminates the surface gravity wave restriction on the timestep. This permits larger timesteps during a simulation resulting in decreased computational time. As a result, the model can easily simulate longterm water quality responses. Version 3.0 will eliminate the diffusion criteria from stability requirements allowing for even larger timesteps.

Head boundary conditions. The model can be applied to estuaries, rivers, or portions of a waterbody by specifying upstream or downstream head boundary conditions.

Multiple branches. The branching algorithm allows application to geometrically complex waterbodies such as dendritic reservoirs or estuaries.

Variable grid spacing. Variable segment lengths and layer thicknesses can be used allowing specification of higher resolution where needed.

Water quality independent of hydrodynamics. Water quality can be updated less frequently than hydrodynamics thus reducing computational requirements. However, water quality kinetics are *not* decoupled from the hydrodynamics (ie., separate, standalone code for hydrodynamics and water quality where output from the hydrodynamic model is stored on disk and then used to specify advective fluxes for the water quality computations). Storage requirements for long-

term hydrodynamic output to drive the water quality model are prohibitive for anything except very small grids. Additionally, reduction in computer time is minimal when hydrodynamic data used to drive water quality are input every timestep.

Autostepping. The model includes a variable timestep algorithm ensuring numerical stability requirements for the hydrodynamics imposed by the solution scheme are not violated.

Restart provision. The user can output results during a simulation that can subsequently be used as input. Execution can then be resumed at that point.

Layer/segment addition and subtraction. The model will adjust surface layer and upstream segment locations for a rising or falling water surface during a simulation.

Multiple inflows and outflows. Provisions are made for inflows and inflow loadings from point/nonpoint sources, branches, and precipitation. Outflows are either specified as releases at a branch's downstream segment or as lateral withdrawals. Although evaporation is not considered an outflow in the strictest sense, it can be included in the water budget.

Ice cover calculations. The model can calculate onset, growth, and breakup of ice cover.

Selective withdrawal calculations. The model can calculate the vertical extent of the withdrawal zone based on outlet geometry, outflow, and density.

Time-varying boundary conditions. The model accepts a given set of time-varying inputs at the frequency they occur independent of other sets of time-varying inputs.

Outputs. The model allows the user considerable flexibility in the type and frequency of outputs. Output is available for the screen, hard copy, plotting, and restarts. The user can specify what is output, when during the simulation output is to begin, and the output frequency. The present version requires the user to develop output plotting/visualization capabilities. Version 3.0 will include X-Windows based pre- and postprocessors for plotting/visualization.

Details of these capabilities are discussed in Appendix C.

Limitations

Theoretical

Hydrodynamics and transport. The governing equations are laterally and layer averaged. Lateral averaging assumes lateral variations in velocities, temperatures, and constituents are negligible. This assumption may be inappropriate for large waterbodies exhibiting significant lateral variations in water quality. Whether this assumption is met is often a judgement call on the user and depends in large part on the questions being addressed.

Eddy coefficients are used to model turbulence. The equations are written in the conservative form using the Boussinesq and hydrostatic approximations. Since vertical momentum is not included, the model may give inaccurate results where there is significant vertical acceleration.

Water quality. Water quality interactions are by necessity simplified descriptions of an aquatic ecosystem that is extremely complex. This is one area in which improvements will be made in the future as better means of describing the aquatic ecosystem in mathematical terms and time for incorporating the changes into the model become available. Many of these limitations will be addressed in Version 3.0. The following list describes the major assumptions in the water quality algorithms.

a. **One algal compartment.** The model includes only one algal compartment and thus cannot model algal succession. In particular, temperature dependency for different algal groups and nitrogen fixation for blue-greens is not modeled. Additional algal groups (diatoms, greens, and blue-greens) will be added in Version 3.0.

b. **No zooplankton.** The model does not explicitly include zooplankton and their effects on algae or recycling of nutrients.

c. **No macrophytes.** The model does not include the effects of macrophytes on water quality. In many cases, this is a good assumption.

d. **Simplistic sediment oxygen demand.** The model does not have a sediment compartment that models kinetics in the sediment and at the sediment-water interface. This places a limitation on long-term predictive capabilities of the water quality portion of the model. If sediments are modeled, then the model is more predictive; however, sediment oxygen demand is still modeled in a simplistic manner. A fully predictive

sediment model that includes carbon diagenesis will be included in Version 3.0.

Numerical

Solution scheme. The model provides two different numerical transport schemes for temperature and constituents - upwind differencing and the higher-order QUICKEST (Leonard, 1979). Upwind differencing introduces numerical diffusion often greater than physical diffusion. The QUICKEST scheme reduces numerical diffusion, but in areas of high gradients generates overshoots and undershoots which may produce small negative concentrations. An option to eliminate overshoots and undershoots will be included in Version 3.0. In addition, discretization errors are introduced as the finite difference cell dimensions or the timestep increase. This is an important point to keep in mind when evaluating model predictions that are spatially and temporally averaged versus observed data collected at discrete points in time and space. A more thorough discussion of the numerical solution and its implementation is found in Appendix A, beginning at page A14 and Appendix D, beginning at page D19.

Computer limits. A considerable effort has been invested in increasing model efficiency. However, the model still places computational and storage burdens on a computer when making long term simulations. In Version 2.0, most of the computations are now performed using single precision (32 bits) but double precision is still needed for some computations. A computer having a minimum of 32 bits of accuracy for single precision arithmetic *must be used*. Year long water quality simulations now typically take from one to three hours of CPU time on a 66Mhz 80486 PC.

Input Data

The availability of input data is not a limitation of the model itself. However, it is most often the limiting factor in the application or misapplication of the model. This cannot be stressed enough. The user should always keep in mind the adage "garbage in equals garbage out".

3 Model Application

This chapter is intended to present the user with a general overview of the steps involved in a model application. The initial user should read the chapter once to gain a general understanding of these steps setting aside questions which may arise upon initial reading. The user should then reread the chapter turning to the additional page references to clarify any questions which arose during the first reading. Filenames are referred to generically (ie., inflow file, outflow file, withdrawal file). Actual filenames are specified by the user in the control file (see pages C107-C137).

Data Preparation

The following data are needed for model application:

    a. geometric data
    b. initial conditions
    c. boundary conditions
    d. hydraulic parameters
    e. kinetic parameters
    f. calibration data

A detailed discussion of these data follows.

Geometric Data

The first input task involves assembling geometric data. These data will be used to define the finite difference representation of the waterbody. The following data are needed for setting up input geometry:

    a. topographic map and/or sediment range surveys
    b. project volume-area-elevation table

The topographic map or sediment range surveys are used to generate bathymetric cross-sections that are input into the model. The project volume-area-elevation table is used for comparison with the volume-area-elevation table generated by the model.

Computational grid. The computational grid is the term used for the finite difference representation of the waterbody. Grid geometry is determined by three parameters:

    a. longitudinal spacing   [DLX]
    b. vertical spacing   [H]
    c. average cross-sectional width   [B]

The longitudinal and vertical spacing may vary from segment to segment and layer to layer but should vary *gradually* from one segment or layer to the next to minimize discretization errors.

Factors affecting computational grid. A number of factors must be evaluated and weighed against each other when determining longitudinal and vertical spacing. These include:

    a. **Areas of strongest gradients.** This factor applies particularly to the metalimnion in freshwater and the pyncnocline in saltwater. If the model is not capturing water quality gradients in these regions, then vertical resolution may have to be increased. Similar reasoning applies to areas of longitudinal gradients.

    b. **Computational and memory requirements.** The model penalizes the user in two ways when increasing grid resolution. As the number of grid cells goes up, so do computational and memory requirements. In addition, as the dimensions of a grid cell decrease, the timestep must also decrease to maintain numerical stability. As a rule of thumb, it is always desirable to err on the side of greater grid resolution, but at some point the user must give way to the reality of the available computer resources and the money and time available for completing the project.

    c. **Bottom slope.** The waterbody bottom slope is more accurately modeled as the ratio of cell thickness to cell length [H]/[DLX] approaches the overall bottom slope.

Previous applications have used a horizontal grid spacing of 100 to 5,000 m and a vertical grid spacing of 0.2 to 5 m.

Bathymetric data. The next step after determining horizontal and vertical cell dimensions is to determine average cross-sectional widths for each cell. This is an iterative procedure whereby initial bathymetry is input into the preprocessor and the volume-area-elevation table is then generated by the preprocessor. This

table is compared to the project table and widths are adjusted to better match the project table.

Several methods have been used for determining average widths. GEDA (Hydrologic Engineering Center, 1981) is a computer program that uses as input cross-sectional data taken at varying longitudinal distances and outputs widths as a function of elevation. The output can then be used to produce bathymetric data for input into CE-QUAL-W2.

Alternatively, transects along the waterbody centerline can be drawn on a topographic map. A contour at the elevation corresponding to the *center* of a grid cell is located and the area encompassed by the contour line and the upstream and downstream transect is determined by planimeter. This area divided by the segment length is the average width of the grid cell. The process is repeated for each grid cell.

When no topographic information is available, the user can determine average widths from sediment range surveys for existing waterbodies. However, this method is generally not as accurate as data obtained from topographic maps since the number of available transects are usually insufficient to adequately describe the complex shape of most waterbodies. If available, sediment range surveys should be used to refine the grid generated from topographic information - particularly where significant sedimentation has occurred.

Sample computational grid. A sample computational grid in the longitudinal/vertical plane with three branches is shown in Figure 1. The FORTRAN variables associated with the grid are also included. The grid consists of 20 longitudinal segments [IMP] and 22 vertical layers [KMP]. They constitute the total number of cells in the computational grid. This is exactly how the model sees the grid layout even though this is not the correct physical representation of the system. In reality, branch two and branch three join branch one. Branch setup is described in more detail below.

Grid cell types. Figure 1 contains two kinds of cells - ones with either a single or a double line border. Cells with a single line border represent cells that may contain water during the simulation. The *active cells* are defined in the bathymetry input as having *non-zero widths*. Cells with a double border represent boundary cells located at or beyond the waterbody boundaries. The *boundary cells* are defined in the bathymetry input as having *zero widths*.

Boundary cells. There are four types of boundary cells:

a. top   c. upstream
b. bottom   d. downstream
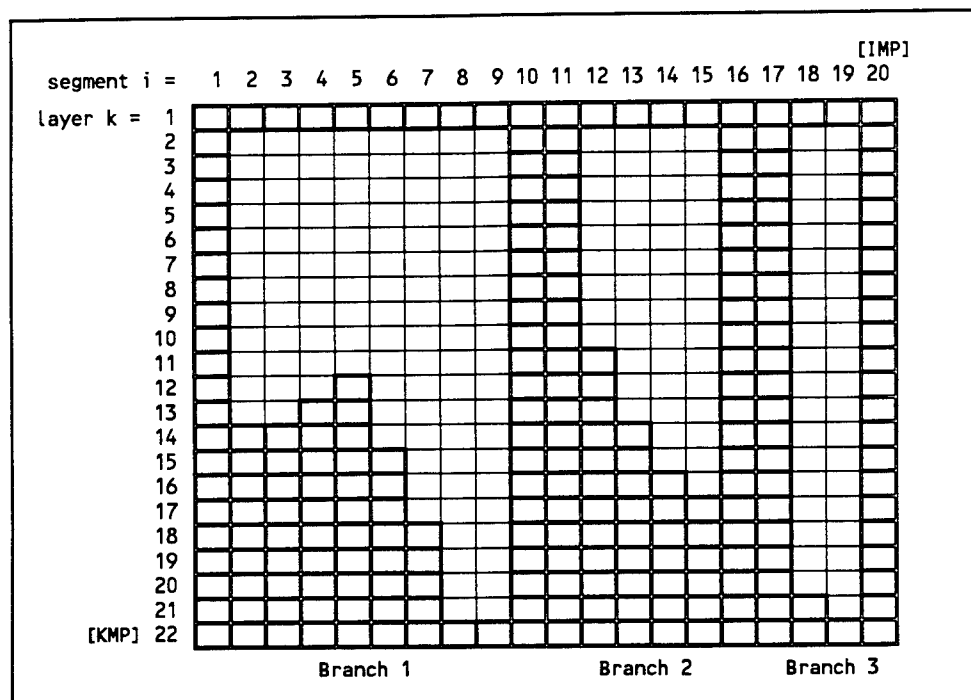
Figure 1. Schematic of three branch CE-QUAL-W2 grid.

Each segment must have a zero width for the cell in layer 1 and a zero width for every cell located below the bottom active cell. For example, cells 1 and 12-22 in segment five would have zero widths. In addition, each branch must have zero widths for upstream boundary and downstream boundary segments. Note this requirement results in *two segments* of boundary cells between each branch (segments 10-11 & 16-17).

Branches.   CE-QUAL-W2 can simulate a waterbody with any number of branches.   Figure 2 shows a plan view of the same three branch grid of Figure 1 along with the FORTRAN variables defining the geometry for each branch.   For each branch, the upstream segment [US] and the downstream segment [DS] must be defined.   The current upstream segment [CUS] is calculated by the model and may vary over time to meet restrictions imposed by the solution scheme (see *a* under **Grid Restrictions**).

A branch may connect to other branches at its upstream [UHS] or downstream segment [DHS].   In Figure 2, the downstream segment of branch 2 ([DS]=15) connects to branch 1 at segment 3 ([DHS]=3).
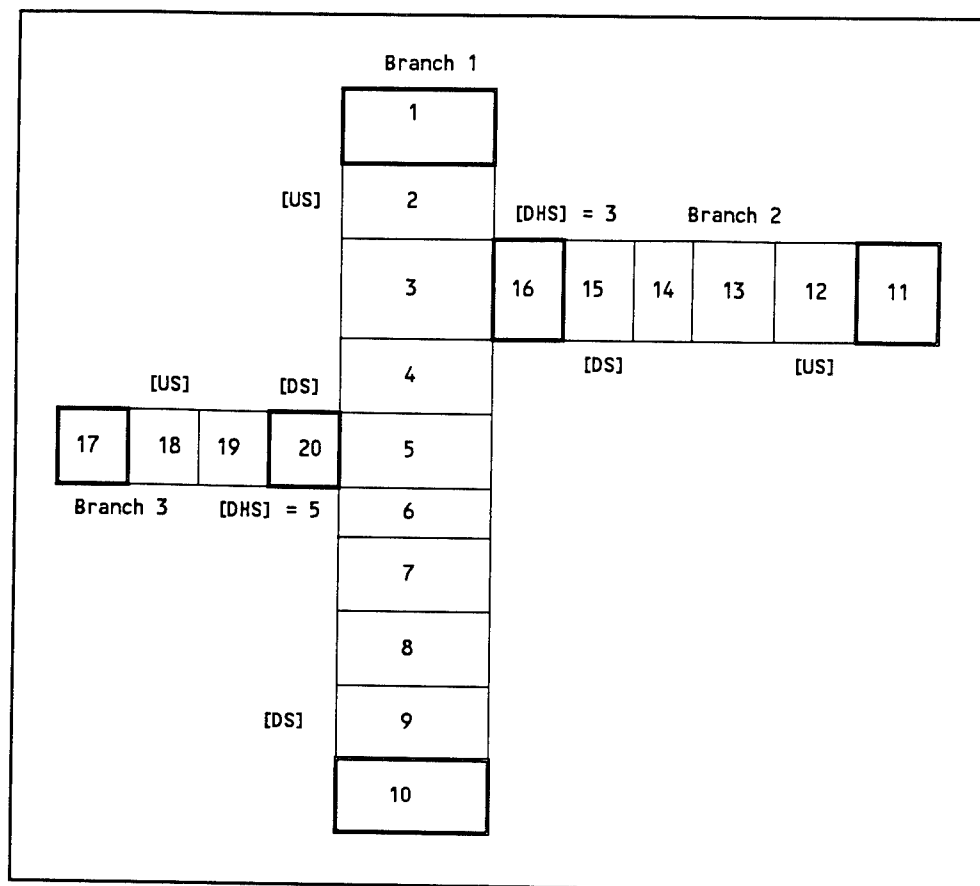
Figure 2. Planar view of CE-QUAL-W2 sample grid.

Grid restrictions. The grid must satisfy the following restrictions:

a. It must be *at least two* active cells deep at every segment. The model ensures this criterion is met during a simulation by adding or subtracting segments.

b. Cell widths *cannot increase* with depth.

c. A branch may connect to other branches at its upstream or downstream segment, but a branch *may not enter or leave* itself.

d. Two branches may not connect at the same segment of another branch.

The bathymetry input file contains the longitudinal grid spacing [DLX], initial water surface elevation [Z], segment orientations [PHI0], vertical grid spacing [H], and average cell widths [B] (see page C146).

After the bathymetry is generated, it should be checked to ensure the bottom elevation varies smoothly and represents the average slope over appropriate portions of the waterbody. Oftentimes, minimum bottom widths are set at from 10-30m. This helps increase timesteps with minimal impact on the volume-area-elevation curves. However, increasing widths in the bottom layers can affect water quality since sediment oxygen demand and nutrient fluxes are dependent on bottom surface areas. Refer to the bathymetry files and prepro-cessor output in the sample applications for additional guidance in setting up the bathymetry.

Initial Conditions

Initial conditions are specified in the control, bathymetry, and vertical and/or longitudinal profile input files. The control file specifies the following initial conditions:

a. **Time.** Starting [TMSTRT] and ending time [TMEND] of the simulation (see page C3).

b. **Temperatures and concentrations.** The initial temperature [IT2] (see page C11) and constituent concentrations [IC2] (see page C73). If the grid is *not* initialized to a single value, then a grid-wide vertical profile can be specified in the vertical profile input file [VPRFN]. The option is also available to specify a longitudinally and vertically varying initial concen-tration for temperature and constituents via the longitudinal profile file [LPRFN].

c. **Inflows/outflows.** The number and location of inflows and outflows (see pages C24-C34).

d. **Restart.** If a previous run with the model was made specify-ing restart conditions were to be written [RSOC] to an output file, then the user can specify the model read the file [RSIC] and continue the simulation from that point (see pages C66-C68).

e. **Waterbody type.** The waterbody can be specified as either saltwater or freshwater [WTYPE] (see page C11).

f. **Ice thickness.** The initial ice thickness [IICETH] (see page C11).

Boundary Conditions

Inflows. The model recognizes the following inflows:

a. **Upstream inflows** (optional). Upstream inflows occur only at a branch's current upstream segment [CUS] which may vary during a simulation. The model provides the option to distribute inflows evenly throughout the inflow segment or place inflows according to density [PQC] (see page C12). *If* the upstream inflow option is used, then a separate file for inflow [QIN], a separate file for temperature [TIN], and, *if* constituents are modeled, a separate file containing constituent concentrations [CIN] for *each* branch is required (see page C152).

b. **Tributary inflows** (optional). Tributary inflows or point source loadings [QTRIB] may enter any segment of the computational grid. If the current upstream segment [CUS] number is greater than the segment the tributary enters, then the tributary inflows are added into the current upstream segment to maintain the waterbody water balance. As in upstream inflows, the model provides the option to distribute tributary inflows evenly throughout the inflow segment or place inflows according to their density [PQTR] (see page C12). The number of tributaries [NTRIB] and their segment location [ITRIB] are specified in the control file (see pages C35-C37). *If* this option is used, then file requirements for *each* tributary are the same as for upstream inflows (see pages C155-C157).

c. **Distributed tributary inflows** (optional). Distributed tributary inflows or nonpoint source loadings [DTRC] may be specified for any branch. The flow is distributed throughout a branch weighted by segment surface areas. *If* this option is used, then file requirements for *each* distributed tributary are the same as for upstream inflows (see pages C158-C160).

d. **Precipitation** (optional). Precipitation [PRC] can be specified for each branch and is distributed according to the segment surface areas (see page C12). *If* this option is used, then file requirements for *each* branch are the same as for upstream inflows (see pages C161-C163).

Outflows. The model recognizes the following outflows:

a. **Downstream outflows** (optional). Downstream outflows [QOUT] occur only at the downstream segment [DS] of a branch. There are two options for specifying downstream outflows. The first is the selective withdrawal option [SWC] where the vertical extent of and flow distribution in the withdrawal zone is calculated by the model (see pages C24-C29). The second allows the user to specify outlet layers where outflow occurs. The number of outlets [NOUT] for each branch and the layer location [KOUT] for each outlet are specified in the control file (see pages C30-C31). For both options, no outflow is allowed to occur if the outlet location is above the current water surface layer [KT]. *If* this option is used, then a separate file for *each* branch is required (see page C153).

b. **Lateral withdrawals** (optional). Lateral withdrawals [QWD] may be specified for any active cell. The number of withdrawals [NWD], their segment location [IWD], and their layer location [KWD] must be specified in the control file (see pages C32-C34). *If* this option is used, a separate file for *each* withdrawal is required (see page C154). Version 3.0 will compute selective withdrawal for lateral withdrawals.

c. **Evaporation** (optional). Evaporation is calculated by the model from air [TAIR] and dewpoint [TDEW] temperature and wind speed [WIND]. If a waterbody loses a significant amount of water from evaporation which is not accounted for in the inflows, then the user should include evaporation. Evaporative heat loss is *always* included in the heat budget.

Head Boundary Conditions (optional). The model recognizes the following head boundary conditions:

a. **External.** The user may specify an external upstream and/or downstream head boundary condition for each branch (see page C8). This boundary specification is intended primarily for estuarine simulations although it has also been used for river and reservoir applications. *If* this option is used, a separate file for time-varying elevations, [EUH] and/or [EDH], a separate file for vertical temperature profiles, [TUH] and/or [TDH], and, if constituents are modeled, a separate file containing vertical profiles for each constituent modeled, [CUH]

and/or [CDH], *must* be specified for *each* external head boundary condition (see pages C164-C167).

b. **Internal**.   Internal head boundary conditions are specified wherever one branch connects with another branch (see page C8). The boundary surface elevation, temperatures, and constituent concentrations are calculated internally by the model.

Surface Boundary Conditions (required). The model requires the following surface boundary conditions:

a. **Surface heat exchange**. Surface heat exchange is calculated by either of two methods using the input variable [HEATC] in the control file (see page A21, C17). The first method uses equilibrium temperatures [ET] and coefficients of surface heat exchange [CSHE] to calculate surface heat exchange (Brady and Edinger, 1975). The second method uses a term-by-term accounting for calculating surface heat exchange. For both methods, latitude [LAT] and longitude [LONG] are specified in the control file (see page C10) and values for air temperature [TAIR], dew point temperature [TDEW], wind speed [WIND] and direction [PHI], and cloud cover [CLOUD] *must* be included in the meteorologic file (see page C149).

b. **Solar radiation absorption**. Distribution of solar radiation in the water column is controlled by the fraction of solar radiation absorbed in the surface layer [BETA] and the attenuation rate due to water [EXH2O], inorganic suspended solids [EXINOR], and organic suspended solids [EXORG].   Values for [EXINOR] and [EXORG] affect solar radiation only if constituents are modeled. These values are specified in the control file (see page C79).

c. **Wind stress**. Wind speed [WIND] and direction [PHI] must be supplied in the meteorologic file [METFN]. Wind stress is an extremely important physical process and should be included in all applications. The model allows the user to specify a wind sheltering coefficient [WSC] which, when multiplied with the wind speed, reduces effects of the wind. The sheltering coefficient is specified in the control file (see pages C20-C22).

d. **Gas exchange**. The wind speed [WIND] supplied in the meteorologic file is also used for computing gas exchange at the water surface if dissolved oxygen and/or total inorganic carbon are simulated (see page C149). Gas exchange is also affected by the wind sheltering coefficient [WSC].

Temperature transport cannot be turned off in the model. Temperature can be treated conservatively by turning off heat exchange computations [HEATC] (see page C16).

Hydraulic Parameters (required)

Dispersion coefficients. The horizontal dispersion coefficients for momentum [AX] and temperature/constituents [DX] are specified in the control file. They are presently time and space invariant. Sensitivity analyses on numerous applications have shown the model is insensitive to variations in the default values. The vertical dispersion coefficients for momentum [AZ] and temperature/constituents [DZ] vary in space and time and are computed by the model.

Chezy coefficient. The Chezy coefficient [CHEZY] is specified in the control file. It is used in calculating boundary friction which varies spatially as a function of exposed bottom area and temporally as a function of the flow field (see page C23). The model does not presently allow for spatially varying Chezy coefficients although Version 3.0 will include this capability.

Kinetic Parameters (optional)

There are approximately 60 coefficients affecting constituent kinetics. The values are specified in the control file. If simulations include water quality, then the user should see Appendix C (pages C79-C106) for a detailed discussion of these coefficients.

Calibration Data (required)

Calibration data are used to provide boundary conditions and assess model performance during calibration. A great deal of thought should go into assessing the amount and type of data necessary to adequately characterize and understand the limnology of a waterbody and to develop the database required to support a water quality modeling effort. Gaugush (1986; 1987; 1993) provides detailed information on sampling design and frequency. *Determining the availability of adequate calibration data should be done as early in the study as possible.* If the user determines calibration data are inadequate, then immediate steps should be taken to collect sufficient data. Results will be suspect at best and will not withstand scrutiny at worst if the model is applied with insufficient and/or inadequate calibration data. The following discussion provides an overview of data required for the proper application of CE-QUAL-W2.

In-Pool. Proper application of mechanistic water quality models requires at least one set of in-pool observed data. The preferred method is *at least* two sets of data encompassing different extremes in the prototype (i.e., high and low

flow years, warm and cold years, spring algal bloom and no spring algal bloom, etc.). In-pool data is used to set initial conditions and assess the model's ability to reproduce observed conditions.

Time-Varying Boundary Conditions. It cannot be overemphasized that data used to drive the model needs to be as accurate as possible. For temperature calibration, this typically means developing regression relationships for inflow temperatures based on flow and air or equilibrium temperature to generate at least daily inflow temperatures (see Ford & Stein, 1984). Equilibrium temperature is preferred since it includes more of the mechanisms affecting water temperature.

For meteorologic data, use the most frequent data available. Previously, daily average values were used to drive the model because earlier 1-D models used daily timesteps. Many modelers still take hourly or three-hourly data and generate daily averages for model input. Any time data is averaged, information is lost. For most reservoirs, thermocline depth and shape are a function of two physical mechanisms - wind mixing and convective cooling. Using daily average air temperatures eliminates nighttime convective mixing which can be a very important physical process affecting epilimnetic depths and thermocline shapes for reservoirs. As another example, applying a daily average wind speed and direction can generate an artificial water surface slope which incorrectly drives hydrodynamics.

For water quality simulations, it is imperative the user provide accurate initial and time-varying boundary conditions. If nutrient loadings are not adequately characterized, then it will be impossible for the model to accurately reproduce algal/nutrient/DO dynamics. It is a waste of time and effort to collect in-pool data in support of water quality modeling when loadings have not been adequately characterized since they often drive the system. As in the development of inflow temperatures, regressions relating loadings with flow and possibly season should be developed for inflowing tributaries. Ideally, several storm events should be intensively sampled since this is when loadings are generally highest to a waterbody. Also, point source loadings should be identified and loading estimates obtained. Some estimate of non-point source loadings should also be made. In some cases, meteorologic loading estimates should be obtained. A software package, FLUX (Walker, 1986), is useful for generating loadings over time from intermittent samples. Table 1 gives general guidelines for data collection.

Kinetic Rates. Because water quality modeling is still very much an art with numerous rate coefficients available for adjustment during calibration, it is highly preferable to obtain actual measurements of these coefficients used in the water quality formulations. If all of the rate coefficients have been determined

for a waterbody, then any discrepancies between computed and observed data highlight the model's shortcomings, help to identify the bounds of the model's predictive capabilities, and provide direction for efficient use of resources to provide a better understanding of the system's water quality dynamics.

Ideally, a model should be used as a starting point for limnological investigations of a waterbody, with the data and formulations continuously refined to reflect the increased understanding of the system and processes gained over time. Unfortunately, this approach is rarely taken in practice due in large part to the expense involved, but also, even more unfortunately, due to the inability of aquatic biologists/limnologists and engineers to collaborate together.

This cooperative approach between experimentalists and theoreticians is the main impetus behind the tremendous advances in physics, chemistry, and, to some extent, biology (eg., genetic research) during the last century, but is seldom seen in the field of water quality modeling. A notable exception is the Chesapeake Bay Modeling Study (Cerco and Cole, 1994). Researchers in the Chesapeake Bay region (both biologists and engineeers) were actively involved in data acquisition and water quality formulations and provided invaluable knowledge and feedback during the course of the study. This cooperative arrangement is continuing and should be a model for all future water quality model development.

Table 1. General guidelines for in-pool water quality sampling.

Boundary Conditions		
Minimum parameters	**Additional parameters**	**Frequency**
inflow/outflow temperature	conductivity dissolved oxygen pH total dissolved solids [1]	daily or continuous
total organic carbon	dissolved and/or particulate organic carbon BOD [2]	weekly w/ storm sampling
soluble reactive phosphorous total phosphorous	total dissolved phosphorus total inorganic phosphorus dissolved inorganic phosphorus	weekly w/ storm sampling
nitrate + nitrite nitrogen ammonium nitrogen	total Kjeldahl nitrogen filtered total Kjeldahl nitrogen	weekly w/ storm sampling
	total suspended solids [3] inorganic and/or volatile suspended solids	weekly w/ storm sampling
	chlorophyll *a* dissolved silica [4] alkalinity	weekly w/ storm sampling

In-Pool		
Minimum parameters	**Additional parameters**	**Frequency**
Temperature[5] Dissolved oxygen[5] pH[5] Conductivity[5]	total dissolved solids [1]	monthly [6]
Chlorophyll a[7]	algal biomass and type	monthly
Total organic carbon[7]	dissolved and/or particulate organic carbon BOD [2]	monthly
Soluble reactive phosphorus Total phosphorus[7]	total dissolved phosphorus total inorganic phosphorus dissolved inorganic phosphorus	monthly
nitrate + nitrite nitrogen ammonium nitrogen[7]	total Kjeldahl nitrogen filtered total Kjeldahl nitrogen	monthly
	secchi depth/light transmission	monthly
	total inorganic carbon alkalinity	monthly
	total suspended solids [3] inorganic and/or volatile suspended solids	monthly
	dissolved/total iron [8] dissolved/total manganese [8] dissolved/total silica [8] total dissolved sulfide [8] sulfate [8] iron sulfide [8]	monthly

[1] enough samples to correlate to conductivity - important for density effects
[2] used to characterize decay rates of organic matter
[3] suspended solids affect phosphorus partitioning, light penetration, and density
[4] can be limiting for diatom growth
[5] preferably bi-weekly - samples should be taken at 1m intervals
[6] 1m intervals
[7] minimum number of samples includes one each in epilimnion, metalimnion, and hypolimnion
 - preferred number of samples (depending on depth) would be at 3m intervals with more frequent metalimnetic sampling
[8] when concerned about sediment release during anoxic periods

Simulations

Once the necessary data have been assembled into proper input format, then simulations can begin. This section describes the recommended steps for obtaining meaningfull model results.

Model Preparation

The amount of application specific modifications to CE-QUAL-W2 have been kept to a minimum. Nonetheless, because of limitations imposed by FORTRAN, *certain modifications must be made to the program*. They are located in the file "W2.INC" and are identified by an exclamation point (!) in column 73 along with a description of what needs to be changed. They include the following:

a. **Control file specification.** The control file [CONFN] may be renamed if the user does not want to use the default - W2_CON.NPT. All other input files are specified in the control file and can be changed without recompiling the program.

b. **PARAMETER statement.** The following parameters may need to be changed:

1) Number of segments   [IMP]
2) Number of layers   [KMP]
3) Number of constituents segments [IMC]
4) Number of constituent layers   [KMC]
5) Number of branches   [NBP]
6) Number of outlet structures   [NSP]
7) Number of tributaries   [NTP]
8) Number of withdrawals   [NWP]
9) Number of output dates   [NDP]

The number of segments [IMP] and layers [KMP] *must always match* the maximum number of segments and layers in the bathymetry file (including boundary layers and segments). The number of constituent segments [IMC] and layers [KMC] are set equal to [IMP] and [KMP] *if* water quality constituents are being simulated. Otherwise, the user should save memory by setting these values to one.

If modifications are made to the include file, then the code *must be recompiled.*

Input checks. Version 2.0 includes a preprocessor program, PRE.FOR, which performs checks of the control file for many errors that can be detected by the preprocessor. Errors are written to the file PRE.OPT and warnings are written to the file PRE.WRN. If no errors are detected, then input from the control file is written to an output file (PRE.OPT). The user should check preprocessor output against inputs to ensure they are correct. Further evaluation of control file input data must be performed by the user to ensure data the user thinks he has input into the model is what the model is actually receiving.

Additionally, **all** time-varying input data should be plotted and screened for errors.

Calibration

The next step is to begin calibration runs. Much of the literature refers to this step as calibration and verification in which model coefficients are adjusted to match an observed data set (calibration) and then the model is run on another data set without adjusting model coefficients to see if the model reproduces observed data in the prototype (verification, confirmation, validation, substantiation, etc.).

This separation is artificial and wrong. If a model does not reproduce observed data (and, more importantly, trends in data) for the "verification" data, then any good modeler will adjust coefficients, review model assumptions, include new processes, or collect additional data to adequately match both sets of data. Often, application to additional sets of data improves the fit to the first. The artificiality of this concept has led to applications in which modelers have used May, June, and July data for "calibration" and August, September, and October data of the same year for "verification" so they can state the model has been "calibrated/verified".

Ideally, calibration should involve multiple data sets encompassing as many variations and extremes as possible in the prototype. A model's ability to reproduce prototype behavior under a variety of conditions gives the modeler more confidence in the model's ability to make predictions under future conditions. To put it very simply, a model is a theory about behavior in the real world. A theory is continuously tested against experimental and/or observed data, and, if it does not match the data, then the theory should either be modified or a new one developed that more closely agrees with observed data.

Model data/comparison. At this stage, the user should have developed some means of displaying output from the model along with observed data. This is a recognized shortcoming of the present version. An X-windows based pre- and postprocessor is presently under development and will be available in Version 3.0. Plotted output is used to interpret model output. Output files available for plotting along with a brief description of their use are given below.

    a. **Profile file [PRFFN].** This file is used to plot observed versus predicted vertical profiles for temperature and constituents at a given segment (see pages C49-C51).

    b. **Time series file [TSRFN].** This file is used to plot time histories of temperature and constituents for inflows, outflows, and withdrawals. This file also contains information to plot out the

time history of the variable timestep and average timestep (see pages C57-C59).

c. **Contour plot file [CPLFN].** This file is used to plot contours of temperature and constituents along the waterbody length (see pages C63-C65).

d. **Vector plot file [VPLFN].** This file is used to plot velocity vectors determined from horizontal and vertical velocities. The output is useful in analyzing flow patterns in the water-body (see pages C60-C62).

e. **Spreadsheet file [SPRFN].** This file is similar to the profile except the output is suitable for importing into a spreadsheet type database for subsequent plotting (see page C138).

Calibration is an iterative process whereby model coefficients are adjusted until an adequate fit of observed versus predicted data is obtained. Unfortunately, there are no hard and fast guidelines for determining when an adequate fit is obtained. The user must continually ask himself "is the model giving reasonable results based on model formulations, assumptions and input data?". If it is not, then the user must determine if the inability of the model to produce reasonable results is due to the use of the model in an inappropriate manner (ie, hydrostatic approximation is invalid, one algal group is not sufficient to capture algal/nutrient/DO interactions, wind speed function for evaporation is inappropriate for the waterbody, etc.), model formulations are insufficient to describe known prototype behavior, or if input data are insufficient to describe the system dynamics.

Another important point to keep in mind during calibration is that a model may give inadequate results for a given spatial and/or temporal scale, but at another scale may reasonably represent the dynamics of the prototype. For example, the model may fail to predict a shortterm algal bloom but may adequately represent algal production over the summer stratification period. The model may thus be useful in determining a waterbody's longterm response to nutrient loading reductions but be inadequate in addressing shortterm responses to a nutrient reduction strategy. In summary, it is not always necessary for model output to match all of the observed data for the model to provide meaningfull results.

The usual sequence for calibration is to check the water budget first, then calibrate temperature (preferably salinity for estuarine applications), and finally water quality. Keep in mind water quality calibration can affect temperature/salinity calibration (see page 25). A description of each follows.

Water budget. The water budget is checked by comparing predicted reservoir elevations with observed elevations. Errors in the water budget are generated by the following:

a. **Incorrect bathymetry**. The user should carefully check the volume-area-elevation table produced by the model to ensure it closely matches the project volume-area-elevation table. If it does not, then bathymetry should be checked carefully to ensure there are no errors (see page C146). In some cases, additional sediment range surveys may be necessary to adequately define the bathymetry. It may also be necessary to include branches that were not included in the initial bathymetry.

b. **Storm events**. Errors in the water budget due to storm events can be determined by comparing predicted with observed elevations using output from the time series plots. If the error is generated during storm events, then the user should check to see if precipitation must be included and/or if more tributaries need to be included than were originally specified. The user may need to use a hydrologic model to determine inflows during storm events for ungaged tributaries. An alternative method is to apportion inflows for ungaged tributaries based on their watershed areas.

c. **Incomplete inflow data.** A substantial amount of inflow is often unaccounted for when using gaged inflows. The unaccounted inflows can include minor tributary, precipitation, stormwater, and wastewater treatment plant contributions. The distributed tributary option provides the user with a means to account for these contributions. This option distributes inflows into every branch segment weighted by the segment surface area (see page C40).

d. **Evaporation**. If evaporation in the region is significant and is not accounted for in inflows, then it should be included using the evaporation option [EVC] (see page C12).

e. **Seepage**. Seepage gains or losses can be significant for some waterbodies. The model does not explicitly handle seepage at present, but the coding is such that seepage can be readily included in the calculations as an additional rate term in the flow source/sink array [QSS].

Typically, the user will plot observed versus predicted water surface elevations for the simulation period. If discrepancies are found, then they should be

analyzed for the cause of error and adjusted for by using one or more of the above options. Remember to always check assumptions used during the gathering of input data to ensure they do not deviate too far from reality.

Hydrodynamics and temperature/salinity. The earliest mechanistic freshwater models (1D) modeled only temperature. As a result, temperature was the only model prediction that could be used for calibration. Since temperature is affected by surface and bottom heat exchange and is therefore nonconservative, it is not the best parameter for calibrating hydrodynamics. The ideal parameter is salinity which is conservative. However, this is generally feasible only for estuarine applications where salinity is routinely monitored. Dissolved solids are not conservative and are generally *not* a good substitute for salinity during calibration except in waterbodies where the conservative assumption is appropriate.

Coefficients affecting temperature and their default values are given in Table 2. The eddy viscosities, Chezy coefficient, and wind sheltering coefficient directly affect hydrodynamics which affect heat transport (and constituents). The remaining coefficients directly affect temperature which affects hydrodynamics. Of these, the last two coefficients affect temperature only if constituents are modeled. See pages C20-C23 and C79 in Appendix C for a more detailed description of these coefficients and their effects.

Table 2. Model coefficients affecting temperature

Coefficient	FORTRAN Name	Default
Longitudinal eddy viscosity	[AX]	1 m^2 sec^{-1}
Longitudinal eddy diffusivity	[DX]	1 m^2 sec^{-1}
Chezy coefficient	[CHEZY]	70 $m^{\frac{1}{2}}$ sec^{-1}
Wind sheltering coefficient	[WSC]	0.85
Solar radiation absorbed in surface layer	[BETA]	0.45
Extinction coefficient for pure water	[EXH2O]	0.4 m^{-1}
Extinction coefficient for inorganic solids	[EXINOR]	0.01 m^{-1}
Extinction coefficient for organic solids	[EXORG]	0.2 m^{-1}

In addition to the above coefficients, temperature predictions are also affected by mainstem and tributary inflows and inflow temperatures and their placement, outlet and withdrawal specifications, the solution scheme, and bathymetry and meteorologic data. Again, always try to represent the prototype as accurately as possible.

Applications on numerous reservoirs under a wide variety of conditions have shown the model generates remarkably accurate temperature predictions using default values when provided accurate geometry and boundary conditions. The wind sheltering coefficient [WSC] has the most effect on temperature during calibration and should be adjusted first. Previous applications with Version 2.0 varied the wind sheltering coefficient from 0.85 for mountainous terrain to 1.0 for open land. The user should also run sensitivity analyses on the other coefficients to gain a "feel" for how they affect temperature predictions.

Difficulties during temperature calibration can often be traced to the following:

a. **Inflows and Inflow temperatures**. Accurate inflows and inflow temperatures are desirable for all applications, but they are critical for waterbodies with short residence times or during high inflow periods. Temperature calibration will be difficult using monthly inflow temperatures for a waterbody with a one week residence time. Methods exist for generating more frequent inflow temperatures based on flow and meteorologic data (Ford and Stein, 1986), but there is no substitute for actual measurements.

b. **Meteorologic data**. Many difficulties are associated with extrapolating weather station meteorologic data to a waterbody site. Weather stations are typically located in different terrain and at large distances from the prototype. Wind data are often measured at 10m above the ground but in the model are applied at the air/water interface. Frontal movements can occur at different times over the waterbody and meteorologic station resulting in model predictions that are in closer agreement either earlier or later than the actual comparison date. Methods for addressing these problems include adjustment of the wind sheltering coefficient [WSC], use of an alternative meteorologic station, averaging data from several meteorologic stations, separating a waterbody into regions applying data from different meteorologic stations, and comparison of observed data using model output either before or after the observed date. If the user has the luxury of obtaining calibration data before applying the model, portable weather stations exist which can be deployed on the waterbody. Obviously, this is the preferred method.

c. **Outflow data**. The addition of the selective withdrawal algorithm in Version 2.0 has reduced many of the previous problems of accurately representing outflows. However, problems

still arise. In the application of CE-QUAL-W2 to Bluestone
Reservoir, Tillman and Cole (1994) were unable to reproduce
observed temperature stratification without limiting the lower
withdrawal layer. Subsequent investigation showed that with-
drawal was limited by trash accumulation which effectively
acted as a submerged weir. This was a problem generated by
inadequate knowledge of the prototype and not a problem with
the model. Indeed, this is an example of a model giving in-
sight into the behavior of the prototype. The current version
of the model does not include the option of using the selective
withdrawal algorithm for withdrawals. Version 3.0 will in-
clude this option.

d. **Bathymetry**. Several previous applications of the model
encountered difficulties during temperature calibration until the
bathymetry was revisited. Check the assumptions made during
the development of the bathymetry to ensure they are not the
source of the problem. Starting points include grid resolution
which affects the models ability to define sharp thermal gradi-
ents and bottom slope, volume-area-elevation accuracy which
can have a marked effect on hypolimnetic temperatures since
the volumes are generally small near the bottom, and water
surface areas which affect the area available for surface heat
exchange. Branch definition has also been found have a pro-
nounced effect on temperature predictions.

Water quality. Since water quality compartments are coupled, calibration of
one compartment may affect other compartments making calibration difficult.
*An understanding of the processes modeled as well as a knowledge of the
system being simulated is an absolute must if the modeling effort is to suc-
ceed*. A complete description of water quality coefficients along with guidelines
for appropriate values are given in Appendix C, pages C79-C106.

Constituents are grouped into three levels (Table 3). In level **I**, the tracer and
total dissolved solids are conservative while coliform bacteria includes a decay
rate. Level **II** includes constituents affecting algal/nutrient/DO dynamics. In
level **III**, alkalinity and total inorganic carbon are transported by the model and
are thus state variables. Carbonate species and pH are calculated from alkalini-
ty and total inorganic carbon.

Table 3. Constituent levels, constituents, and constituent numbers.

Level	Constituent	Constituent number
I	Tracer	1
	Inorganic suspended solids	2
	Coliform bacteria	3
II	Total dissolved solids (or salinity)	4
	Labile DOM	5
	Refractory DOM	6
	Algae	7
	Detritus	8
	Phosphorus	9
	Ammonium	10
	Nitrate-nitrite	11
	Dissolved oxygen	12
	Sediment	13
III	Total inorganic carbon	14
	Alkalinity	15
	pH	16
	Carbon dioxide	17
	Bicarbonate	18
	Carbonate	19
IV	Iron	20
	CBOD	21

The user should spend time familiarizing himself with the water quality formulations in Appendix B taking note of the assumptions used. During water quality calibration, a process neglected in the formulations may need to be included. For example, carbonate precipitation is not included in the formulations. If phosphorus coprecipitation with calcium carbonate is known to be an important phosphorous removal mechanism, then it should be included. The water quality subroutines are formulated so that additional kinetic relationships can easily be incorporated into the model through additional coding.

Because the model was developed for application to a wide range of waterbodies for a variety of problems, recommending a general procedure for calibrating algal/nutrient/DO dynamics is not possible. Experience is the only way to become proficient at water quality calibration. However, as a starting point, particular care should be paid to the timing and duration of events involving algae and dissolved oxygen. If the onset, extent, and duration of anoxic conditions are not represented by the model, then nutrient dynamics will not be represented either. They in turn affect algal production which affects dissolved oxygen. Much of the art in water quality modeling is involved in calibrating algal/nutrient/DO dynamics.

A few final words about model calibration. For some applications, no amount of model adjustment or data reconstruction will provide acceptable calibration. For these cases, the model can still be used to provide information about the prototype. The model may point out data inadequacies, important mechanisms not included in the model but important in the protoype, or inappropriate assumptions used in the model.

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Appendix A
Hydrodynamics and Transport

Fundamental Equations

CE-QUAL-W2 uses the laterally averaged equations of fluid motion derived from the three dimensional equations (Edinger and Buchak, 1975). They consist of six equations and six unknowns. The equations are:

Horizontal Momentum

$$\frac{\partial UB}{\partial t} + \frac{\partial UUB}{\partial x} + \frac{\partial WUB}{\partial z} = -\frac{1}{\rho}\frac{\partial BP}{\partial x} + \frac{\partial\left[BA_x\frac{\partial U}{\partial x}\right]}{\partial x} + \frac{\partial B\tau_x}{\partial z} \qquad (A-1)$$

where

U = longitudinal, laterally averaged velocity, $m\ sec^{-1}$
B = waterbody width, m
t = time, sec
x = longitudinal Cartesian coordinate: x is along the lake centerline at the water surface, positive to the right
z = vertical Cartesian coordinate: z is positive downward
W = vertical, laterally averaged velocity, $m\ sec^{-1}$
ρ = density, $kg\ m^{-3}$
P = pressure, $N\ m^{-2}$
A_x = longitudinal momentum dispersion coefficient, $m^2\ sec^{-1}$
τ_x = shear stress per unit mass resulting from the vertical gradient of the horizontal velocity, U, $m^2\ sec^{-2}$

The first term represents the time rate of change of horizontal momentum, and the second and third terms are the horizontal and vertical advection of momentum. The first term on the right-hand side (RHS) of equation (A-1) is the force imposed by the horizontal pressure gradient. The second term on the RHS is the horizontal dispersion of momentum, and the third term is the force due to shear stress.

Constituent Transport

$$\frac{\partial B\Phi}{\partial t} + \frac{\partial UB\Phi}{\partial x} + \frac{\partial WB\Phi}{\partial z} - \frac{\partial\left[BD_x\frac{\partial\Phi}{\partial x}\right]}{\partial x} - \frac{\partial\left[BD_z\frac{\partial\Phi}{\partial z}\right]}{\partial z} = q_\Phi B + S_\Phi B \qquad \text{(A-2)}$$

where

Φ = laterally averaged constituent concentration, $g\ m^{-3}$

D_x = longitudinal temperature and constituent dispersion coefficient, $m^2\ sec^{-1}$

D_z = vertical temperature and constituent dispersion coefficient, $m^2\ sec^{-1}$

q_Φ = lateral inflow or outflow mass flow rate of constituent per unit volume, $g\ m^{-3}\ sec^{-1}$

S_Φ = kinetics source/sink term for constituent concentrations, $g\ m^{-3}\ sec^{-1}$

Each constituent has a balance as in equation (A-2) with specific source and sink terms. The first term in equation (A-2) represents the time rate of change of constituent concentration and the second and third terms are the horizontal and vertical advection of constituents. The fourth and fifth terms are the horizontal and vertical diffusion of constituents. The first term on the RHS is the lateral inflow/outflow of constituents, and the second term represents kinetic source/sink rates for constituents.

Free Water Surface Elevation

$$\frac{\partial B_\eta \eta}{\partial t} = \frac{\partial}{\partial x}\int_\eta^h UB\,dz - \int_\eta^h qB\,dz \qquad \text{(A-3)}$$

where

B_η = time and spatially varying surface width, m

η = free water surface location, m

h = total depth, m

q = lateral boundary inflow or outflow, $m^3\ sec^{-1}$

Hydrostatic Pressure

$$\frac{\partial P}{\partial z} = \rho g \qquad \text{(A-4)}$$

where

g = acceleration due to gravity, $m\ sec^{-2}$

Continuity

$$\frac{\partial UB}{\partial x} + \frac{\partial WB}{\partial z} = qB \qquad \text{(A-5)}$$

Equation of State

$$\rho = f(T_w, \Phi_{TDS}, \Phi_{ss}) \qquad \text{(A-6)}$$

where

$f(T, \Phi_{TDS}, \Phi_{ss})$ = density function dependent upon temperature, total dissolved solids or salinity, and suspended solids

The six equations result in six unknowns:

1. free water surface elevation, η
2. pressure, P
3. horizontal velocity, U
4. vertical velocity, W
5. constituent concentration, Φ
6. density, ρ

Lateral averaging eliminates the lateral momentum balance, lateral velocity, and Coriolis acceleration. The solution of the six equations for the six unknowns forms the basic model structure.

Horizontal Pressure Gradient Evaluation

The laterally averaged horizontal pressure gradient in the horizontal momentum balance includes the density driving force. It can be expanded to:

$$\frac{\partial BP}{\partial x} = B\frac{\partial P}{\partial x} + P\frac{\partial B}{\partial x} \tag{A-7}$$

The second term represents the static force of the fluid on the x projection of the lateral boundary, which in turn is cancelled by the force of the boundary on the fluid. Thus, this term represents the internal fluid horizontal pressure gradient. The horizontal pressure gradient is evaluated in combination with equation (A-4) to give:

$$B\frac{\partial P}{\partial x} = -\rho_\eta B g\frac{\partial \eta}{\partial x} + B g \int_\eta^z \frac{\partial \rho}{\partial x} dz \tag{A-8}$$

at any depth z, where ρ_η is the density at the surface. The horizontal pressure gradient is divided into two components - the surface slope and the vertical integral of the horizontal density gradient. The first term is the barotropic gradient and the second is the baroclinic gradient. The horizontal pressure gradient is the major driving force for density circulation in many waterbodies.

Free Water Surface Evaluation

The basic characteristics of longitudinal and vertical free water surface hydrodynamics can be examined through evaluation of equation (A-3). The vertical integral of the horizontal flow can be determined from the algebraic forward-time difference of the local acceleration of horizontal momentum in equation (A-1). Formulation of the forward-time difference of UB, $U'B'$, is the first step in evaluating the numerical equations. It gives:

$$U'B' = UB - \frac{B\Delta t}{\rho}\frac{\partial P}{\partial x} + F_x\Delta t + \Delta tB\frac{\partial \tau_x}{\partial z} \tag{A-9}$$

where

$$F_x = \frac{\partial \left[BA_x\frac{\partial U}{\partial x}\right]}{\partial x} - \frac{\partial UUB}{\partial x} - \frac{\partial WUB}{\partial z} \tag{A-10}$$

The vertical integrals of the various terms in equations (A-9) and (A-10) can be further evaluated for insertion into the vertical integral of the flow required in the free water surface balance, equation (A-3). The vertical integral of the horizontal pressure gradient, the second term on the RHS of equation (A-9), can be evaluated from equation (A-8) to give:

$$\frac{1}{\rho_\eta} \int_\eta^h B \frac{\partial P}{\partial x} dz = -\frac{\partial \eta}{\partial xg} \int_\eta^h B\, dz + \frac{g}{\rho_\eta} \int_\eta^h \left[B \int_\eta^z \frac{\partial \rho}{\partial x} dz \right] dz \qquad (A\text{-}11)$$

The first term on the RHS of equation (A-11) results from the fact that $\partial \eta / \partial x$ is a function only of x and is constant over z. The integral of width B over depth is the total cross-sectional area across which the surface slope contribution to the horizontal pressure gradient acts. The second term is the force due to the horizontal density gradient.

The vertical integral of the horizontal shear stress, the last term on the RHS of equation (A-9), can be expanded from the derivations of $B \partial \tau_x / \partial z$ to give:

$$\int_\eta^h B \frac{\partial \tau_x}{\partial z} dz = B_h \tau_h - B_\eta \tau_\eta - \int_\eta^h \tau_x \frac{\partial B}{\partial z} dz \qquad (A\text{-}12)$$

The first term on the RHS of equation (A-12) is column bottom shear evaluated at $z = h$ and can be evaluated from bottom velocity friction relationships. The surface shear, $B_\eta \tau_\eta$, is the surface wind shear component parallel to the x axis. The third term is wall or bottom shear due to the horizontal projection of the sloping sides of the waterbody. It is evaluated as bottom shear over the projected width at each elevation. The internal velocity shear cancels in the vertical integration.

Collecting the various terms of equation (A-9) into equation (A-3) gives the surface elevation equation of:

$$\frac{\partial B\eta}{\partial t} - g\Delta t \frac{\partial}{\partial x} \left[\frac{\partial \eta}{\partial x} \int_\eta^h B\, dz \right] = \frac{\partial}{\partial x} \int_\eta^h UB\, dz - \frac{g\Delta t}{\rho_\eta} \frac{\partial}{\partial x} \int_\eta^h \left[B \int_\eta^z \frac{\partial \rho}{\partial x} dz \right] dz$$

$$+ \frac{\partial}{\partial x} \left[B_h \tau_h - B_\eta \tau_\eta - \int_\eta^h \tau_x \frac{\partial B}{\partial z} dz \right] \Delta t$$

$$+ \frac{\partial}{\partial x} \left[\int_\eta^h F_x\, dz \right] \Delta t - \int_\eta^h qB\, dz \qquad (A\text{-}13)$$

With the water surface terms (η) collected on the left-hand side, equation (A-13) is the water surface equation of the integrated waterbody. Therefore, equation

(A-13) is a numerical form of the frictionally dampened, longwave equation for a stratified waterbody with an irregular geometry.

Numerical Solution

The first step in the numerical solution is to define the computational grid (Figure A-1). The grid is space-staggered since some variables are defined at one location and the remainder are displaced by $\Delta x/2$ or $\Delta z/2$. The grid discretizes a waterbody into computational cells whose locations are defined by their segment (i) and layer number (k), i.e., cell (k,i). Variables are located at either the center or boundary of a cell. Variables defined at the boundary include the velocities U and W, dispersion coefficients A_x, D_x, A_z, and D_z, and internal shear stress τ_x. The variables ρ, Φ, P, and B are defined at the cell center.
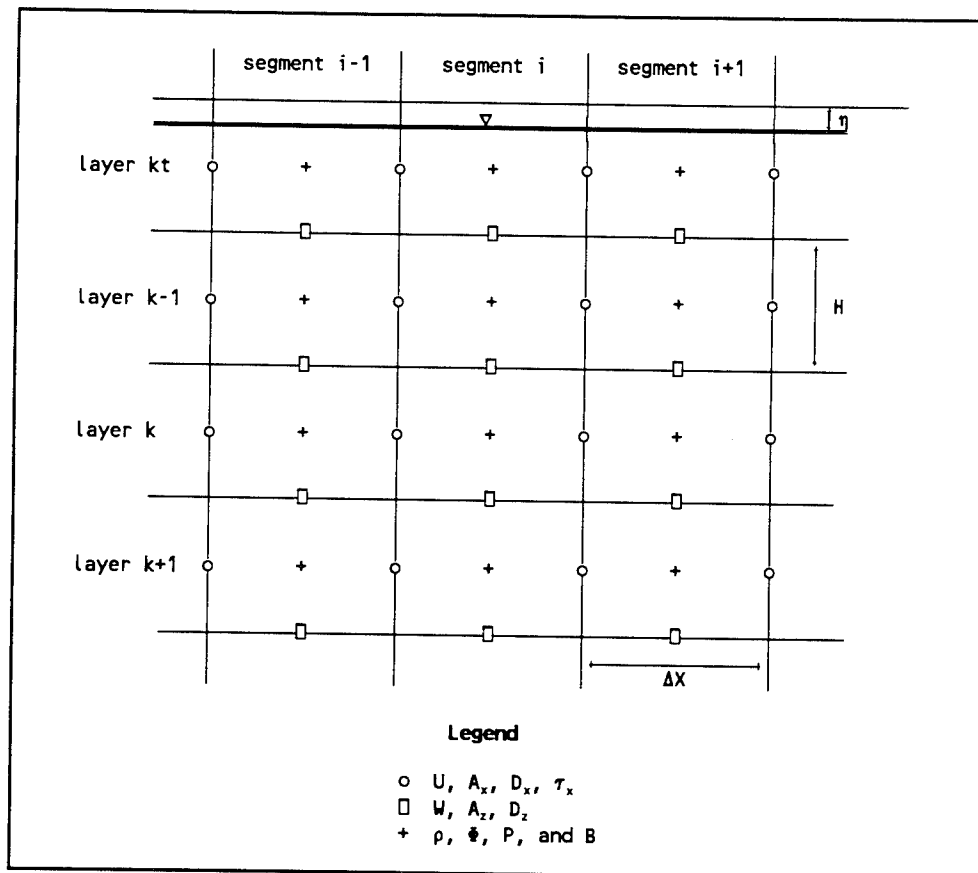
Figure A-1. Variable locations in computational grid.

There is a rational basis for choosing variable locations. Since the constituent concentration is defined at the center and velocities are defined at the boundaries, spatial averaging of velocities is not required to determine changes in concentration over time. Also, the horizontal velocity is surrounded by a cell with water surface elevations and densities defined on either side. Thus, the horizontal velocity is computed from horizontal gradients of the surface slope and densities without requiring spatial averaging of these variables.

The geometry is specified in Figure A-1 by a cell width B, cell thickness H, and cell length Δx. Several additional geometric variables are used in the calculations. These include the average cross-sectional area between two cells (k,i) and (k,i+1)

$$BH_{r_{k,i}} = \frac{B_{k,i} H_{k,i} + B_{k,i} H_{k,i+1}}{2} \tag{A-14}$$

the average widths between two cells (k,i) and (k+1,i)

$$B_{b_{k,i}} = \frac{B_{k,i} + B_{k+1,i}}{2} \tag{A-15}$$

and the average layer thickness between layers k and k+1

$$\overline{H}_{k,i} = \frac{H_k + H_{k+1}}{2} \tag{A-16}$$

The numerical procedure for solving the six unknowns at each timestep is to first compute water surface elevations from equation (A-13). With the new surface elevations, new horizontal velocities can be computed from equation (A-9). With new horizontal velocities, the vertical velocities can be found from continuity, equation (A-5). New constituent concentrations are computed from the constituent balance, equation (A-2). Using new horizontal and vertical velocities, the water surface elevation equation, equation (A-13), can be solved for η simultaneously. The solution for η is thus spatially implicit at the same time level and eliminates the surface gravity wave speed criterion:

$$\Delta t < \frac{\Delta x}{\sqrt{g\, H_{max}}} \tag{A-17}$$

which can seriously limit timesteps in deep waterbodies.

Surface Wave Equation

The numerical form of the surface elevation equation, equation (A-13), can be written in terms of the finite difference grid and its definitions given in Figure A-1. The vertically integrated momentum terms from the wave equation can be written in finite difference layer-averaged form as:

$$F = \frac{-g\,BH_r}{\rho} \int_\eta^z \frac{\partial \rho}{\partial x}\,dz - \frac{\partial(U^2 BH)}{\partial x} - (UWB)_{k+\frac{1}{2}} + (UWB)_{k-\frac{1}{2}}$$

$$+ \frac{\partial \left[BH\,A_x\,\frac{\partial U}{\partial x} \right]}{\partial x} - (\tau_x B)_{k+\frac{1}{2}} + (\tau_x B)_{k-\frac{1}{2}}$$

(A-18)

When computing the new value of η at time n+1, terms in F are evaluated from values at timestep n. The RHS terms in equation (A-18) are:

1. density gradient component of the horizontal pressure gradient
2. gradient of horizontally advected momentum
3,4. vertical advection of momentum into layer k
5. horizontal dispersion of momentum
6. horizontal shear stress on the bottom of layer k
7. horizontal shear stress on the top of layer k

Substitution of the vertically integrated momentum balance into the vertically integrated continuity balance results in the surface wave equation which can be written in time-backward, spatially implicit tridiagonal form as:

$$A_{\eta_i} Z_{i-1} + V_{\eta_i} Z_i + C_{\eta_i} Z_{i+1} = D_{\eta_i}$$ (A-19)

where the tridiagonal matrix coefficients A_η, V_η, and C_η include reservoir geometry summed over a cross-section as:

$$A_{\eta_i} = -g\,\frac{\Delta t^2}{\Delta x} \sum_k BH_{r_{k,i-1}}$$ (A-20)

$$V_{\eta_i} = \Delta x\,B_{k,i} + g\,\frac{\Delta t^2}{\Delta x}\left[\sum_k BH_{r_{k,i-1}} + \sum_k BH_{r_{k,i}} \right]$$ (A-21)

$$C_{\eta_i} = -g\,\frac{\Delta t^2}{\Delta x} \sum_k BH_{r_{k,i}}$$ (A-22)

The A_η geometry is the cross-sectional area between the i-1 and i segments, the C_η geometry is the cross-sectional area between the i and i+1 segments, and the geometry in V_η is the sum of the two cross-sections. The tridiagonal coefficient D_η includes the overall dynamics, inflows, and outflows as:

$$D_{\eta_i} = \Delta x\, B_{kt,i} Z_i + \Delta t^2 \sum_k \left[F_{k,i} - F_{k,i-1} \right]$$
$$+ \Delta t \sum_k \left[U_{k,i} BH_{r_{k,i}} - U_{k,i-1} BH_{r_{k,i-1}} \right] - \Delta t \sum_k Q_{k,i}$$

$$(A\text{-}23)$$

where $Q_{k,i}$ is lateral boundary inflow or outflows at cell k,i. Equation (A-18) is solved using the Thomas tridiagonal algorithm.

Equation (A-18) applies throughout the grid that represents the water body, including boundaries where there is zero flux. To incorporate longitudinal flow boundary conditions, D_η is modified by subtracting total inflow or adding total outflow over a timestep for the left and right boundaries, respectively.

Head boundary conditions are incorporated into the solution by using the off-diagonal coefficients, [A(CUS)] and/or [C(ID)], with boundary elevations specified at the upstream and/or downstream ends of the computational grid. These terms are ordinarily ignored by the Thomas algorithm. However, here they are subtracted from D_η in the solution for upstream and/or downstream surface elevations.

There are two cases in which head boundary conditions are used - open boundaries for which the external head or elevation is known, as in estuaries, and branch boundaries where the applied head is generated by solution of the surface wave equation in a joining branch, as in multistemmed reservoirs. In the latter, the numerical solution is applied to each branch in turn with internal boundary conditions joining the branches. Since branch computations are performed sequentially, calculation accuracy can be increased by numbering branches beginning with the mainstem. The remainder of the branches are numbered beginning with the most upstream branch then proceeding downstream.

Evaluation of Forcing Function Terms

The forcing function in the wave equation, F, in equation (A-18) must be evaluated before water surface elevations are computed at the new timestep. All terms in F are therefore computed from values at the previous timestep. New timestep data entering the wave equation are boundary inflows, outflows, and surface heights. Many of the terms entering F, including the longitudinal

and vertical advection of momentum, longitudinal dispersion of momentum, and horizontal shear also enter the horizontal momentum balance for the U computations and are evaluated and saved as separate arrays.

Contribution of the horizontal density gradient to horizontal momentum is an integral over depth from a fixed reference surface of a horizontal density gradient. It applies at the i to i+1 boundary where U and F are located. The horizontal density gradient is first computed using the vertical integration of pressure as:

$$P_{k,i} = P_{k-1,i} + g\rho_{k,i} H_{k,i} \tag{A-24}$$

which is then used to calculate the horizontal pressure gradient, HPG:

$$HPG_{k,i} = \frac{B_{k,i} + B_{k,i+1}}{\Delta x \rho} \left[H_{k,i+1} P_{k-1,i+1} + P_{k,i+1} - H_{k,i} P_{k-1,i} + P_{k,i} \right] \tag{A-25}$$

Constituent Transport

Version 1.0 used upwind differencing in the constituent transport advective terms in which the cell concentration immediately upstream of the velocity is used to calculate fluxes. A major problem with upwind differencing is the introduction of numerical diffusion given by (for longitudinal advection):

$$\alpha_c = \frac{u\Delta x}{2} (1-c) \tag{A-26}$$

where

α_c = numerical diffusion

$c = \dfrac{U\Delta t}{\Delta x}$

A similar condition holds for vertical advection. In many cases, numerical diffusion can overwhelm physical diffusion producing inaccurate results when strong gradients are present. The problem is particularly pronounced for stratified reservoirs and estuaries.

Numerical diffusion has been reduced by implementing an explicit, third-order accurate QUICKEST horizontal/vertical transport scheme (Leonard, 1979), and

time-weighted, implicit vertical advection. Tests of this scheme are reported in Chapman and Cole (1992).

QUICKEST uses an additional spatial term to estimate concentrations used in computing horizontal and vertical fluxes. A nonuniform grid QUICKEST scheme was developed using a three-point Lagrangian interpolation function to estimate constituent values at grid cell interfaces. Specifically, advective multi-pliers for each of three upstream weighted grid cells are derived in terms of cell lengths and the local cell interface velocity. Time invariant parts of the interpo-lation functions are calculated once thus minimizing computations for additional constituents.

Implicit vertical transport including variable layer heights has also been imple-mented. Vertical diffusion is fully implicit and advection employs a time-weighted, central difference, implicit scheme. A unique feature of vertical advection, in the explicit part of the time-weighted scheme, is QUICKEST which increases overall accuracy.

As implemented in the code, the new transport scheme is a two-part solution for constituent concentrations at the new timestep. First, horizontal advection is computed using QUICKEST and diffusion is computed using central differenc-ing. This part also includes the explicit vertical advection contribution (which utilizes QUICKEST) and all sources and sinks.

Next, the implicit part of vertical advection and diffusion are included. Diffu-sion is always fully implicit. The user can time-weight advection by specifying a value for [THETA] which varies from 0 to 1. For [THETA] equal to 0, the solution is explicit in time and vertical advection is accounted for in the first part of the algorithm. For [THETA] equal to 1, the solution is fully implicit in time and vertical advection is accounted for in this part of the algorithm. A Crank-Nicholson scheme where vertical advection is time-weighted between the explicit (using QUICKEST) and implicit parts results if [THETA] is set to 0.55. The following is a description of the preferred transport scheme - QUICKEST.

Non-Uniform Grid QUICKEST Formulation. In one dimension, the conser-vative control volume advective transport of a constituent Φ integrated over a timestep is:

$$\Phi_i^{n+1} = \Phi_i^n - \frac{\Delta t}{\Delta x}(U_r \Phi_r^n - U_l \Phi_l^n) \qquad \text{(A-27)}$$

where

Φ_i = constituent concentration at a grid point
$\Phi_{r,l}$ = right and left cell face constituent concentrations
$U_{r,l}$ = right and left cell face velocity
t = time

The QUICKEST algorithm was originally derived using an upstream weighted quadratic interpolation function defined over three uniformly spaced grid points. This interpolation function estimates cell face concentrations required by the conservative control volume transport scheme. For example, the right cell face concentration estimate for a flow positive to the right is:

$$\Phi_r = T_{i-1}\Phi_{i-1} + T_i\Phi_i + T_{i+1}\Phi_{i+1} \tag{A-28}$$

where T are advective multipliers which weight the contribution of three adjacent grid point concentrations.

The advective multipliers are obtained by collecting terms associated with each constituent defined by the QUICKEST advection operator. For a non-uniform grid, a combination of two and three point Lagrangian interpolation functions (Henrici, 1964) are used to compute the QUICKEST estimate for the right cell face concentration centered about cells i and i+1:

$$\Phi_r = P_1(x) - \frac{U\Delta t}{2} P_2(x) + \left[D_x\Delta t - \frac{1}{6} \left[\Delta x^2 - (U\Delta t)^2 \right] \right] P_2''(x) \tag{A-29}$$

where

x = the local right cell face position
D_x = diffusion coefficient

Defining a local coordinate system of three non-uniformly spaced grid cells denoted by x_{i-1}, x_i, and x_{i+1} with corresponding constituent values, the interpolation functions required in equation (A-28) are:

$$P_1(x) = \frac{(x-x_i)}{(x_{i+1}-x_i)} \Phi_{i+1} + \frac{(x_{i+1}-x)}{(x_{i+1}-x_i)} \Phi_i \tag{A-30}$$

and

$$P_2(x) = \frac{(x-x_i)(x-x_{i-1})}{(x_{i+1}-x_i)(x_{i+1}-x_{i-1})}\Phi_{i+1} + \frac{(x-x_{i+1})(x-x_{i-1})}{(x_i-x_{i+1})(x_i-x_{i-1})}\Phi_i$$
$$+ \frac{(x-x_{i+1})(x-x_i)}{(x_{i-1}-x_{i+1})(x_{x-1}-x_i)}\Phi_{i-1}$$

(A-31)

Taking the first derivative of $P_1(x)$ and the second derivative of $P_2(x)$ and substituting into equation (A-28), it is then possible to group terms and obtain the advective multipliers. For example, the T_{i+1} multiplier is:

$$T_{i+1} = \frac{(x-x_i)}{(x_{i+1}-x_i)} - \frac{U\Delta t}{2}\frac{\left[(x-x_i)+(x-x_{i-1})\right]}{(x_{i+1}-x_i)(x_{i+1}-x_{i-1})}$$
$$+ \frac{2\left[D_x\Delta t - \frac{1}{6}\left[\Delta x_i^2 - (U\Delta t)^2\right]\right]}{(x_{i+1}-x_i)(x_{i+1}-x_{i-1})}$$

(A-32)

Similar functions are obtained for T_i and T_{i-1} multipliers which completes the formulation for the QUICKEST algorithm.

From a computational standpoint, most geometric components of the multipliers are time-invariant and are computed once and stored in arrays. The time-varying part of the multipliers $(U, \Delta t, D_x)$ are updated each timestep during computation of the T arrays. However, when the QUICKEST scheme is applied vertically, the spatial part of the multipliers for layers KT and KT+1 are updated each timestep to accommodate the surface elevation fluctuation.

Vertical Implicit Transport. Focusing on vertical advective and diffusive transport, constituent transport can be written:

$$\frac{\partial B\Phi}{\partial t} + \frac{\partial WB\Phi}{\partial z} - \frac{\partial}{\partial z}\left[BD_z\frac{\partial \Phi}{\partial z}\right] = RHS$$

(A-33)

where RHS represents horizontal transport, and all sources/sinks. Integrating the transport equation vertically and over time yields:

$$BH\Phi^{n+1} + \theta\Delta t\delta_z(WB\Phi^{n+1}) - \Delta t\delta_z\left[BD_z\frac{\partial\Phi^{n+1}}{\partial z}\right] = BH\Phi^*$$

(A-34)

where

Φ^* = all n-time level horizontal and explicit vertical transport and sources/sinks

θ = time-weighting for vertical advection, 0 if fully explicit, 0.55 if Crank-Nicholson, and 1 if fully implicit

Expanding the differential operators in terms of central differences and collecting terms, equation (A-10) can be recast as:

$$A_{t_i} \Phi_{i-1}^{n+1} + V_{t_i} \Phi_i^{n+1} + C_{t_i} \Phi_{i+1}^{n+1} = D_{t_i} \qquad \text{(A-35)}$$

where

$$A_{t_i} = \frac{\Delta t B_{b_{k,i}}}{BH_{k,i}} \left[\theta \frac{W_{k,i}}{2} - \frac{D_{z_{k,i}}}{H_k} \right] \qquad \text{(A-36)}$$

$$V_{t_i} = 1 + \frac{\Delta t}{BH_{k,i}} \left[\theta \left[\frac{W_{k,i} B_{b_{k,i}} - W_{k-1,i} B_{b_{k-1,i}}}{2} \right] + \frac{B_{b_{k,i}} D_{z_{k,i}}}{H_k} + \frac{B_{b_{k-1}} D_{z_{k-1,i}}}{H_{k-1}} \right] \qquad \text{(A-37)}$$

$$C_{t_i} = - \frac{\Delta t B_{b_{k-1,i}}}{BH_{k,i}} \left[\theta \frac{W_{k-1,i}}{2} + \frac{D_{z_{k-1,i}}}{H_{k-1}} \right] \qquad \text{(A-38)}$$

The coefficients are computed once, stored in arrays, and used to update each constituent. This is accomplished by loading the explicit part of the solution, Φ^*, with each successive constituent and inverting the resulting matrix via a Thomas tridiagonal solver.

Auxiliary Functions

Auxiliary functions are relationships that describe processes independent of basic hydrodynamic and transport computational schemes in the model. Auxiliary functions include turbulent dispersion and wind shear processes, heat exchange (including ice cover), evaporation, density function, and selective withdrawal.

Turbulence and Wind Shear

In two-dimensional longitudinal-vertical models, wind shear enters the longitudinal momentum balance through the vertical transport of horizontal momentum written for the time averaged, instantaneous velocity as $\partial <wu>/\partial z$. The instantaneous horizontal and vertical velocities can be written as:

$$u = U + u' + u''$$ (A-36a)

$$w = W + w' + w''$$ (A-36b)

where

   U and W = time averaged, mean velocity components
   u' and w' = turbulent velocity fluctuations about the mean generated by velocity shear
   u'' and w'' = velocity components of wind waves propagated downward from the water surface

The time mean of the instantaneous velocity product becomes:

$$<uw> = UW + <u'w'> + <u''w''>$$ (A-37)

Turbulent transport is related to the mean velocity as:

$$<u'w'> = -A_z \frac{\partial U}{\partial z}$$ (A-38)

where A_z is the vertical eddy viscosity. Shear due to wind waves can be evaluated from the vertical decay of wind wave velocities given for simple sinusoidal waves as:

$$u'' = A\sigma e^{-kz} \sin(kx - \sigma t)$$ (A-39a)

$$w'' = A\sigma e^{-kz} \sin(kx - \sigma t + \phi)$$ (A-39b)

where

   σ = wave frequency ($2\Pi/T$ where T = wave period)
   ϕ = phase shift between vertical and horizontal components
   σ = ck, where c is the wave speed and k = $2\Pi/L$,
       where L is the wave length

Averaged over time, shear due to velocity fluctuations becomes:

$$<u''w''> = \tau_{wx} e^{-2kz}$$ (A-40)

where

   τ_{wx} = surface shear due to wind along the x-axis of the model

The horizontal shear becomes:

$$\tau_x = -A_z \frac{\partial U}{\partial z} + \tau_{wx} e^{-2kz} \tag{A-41}$$

Thus, wind shear decays with depth and generates horizontal velocities directly through the horizontal momentum balance and momentum is dissipated through the vertical eddy viscosity.

The vertical eddy viscosity for longitudinal-vertical dynamics can be formulated by analogy to the three-dimensional case:

$$A_z = k \left[\frac{l^2}{2} \right] \sqrt{ \left[\frac{\partial U}{\partial z} \right]^2 + \left[\frac{\partial V}{\partial z} \right]^2 } \, e^{(-CR_i)} \tag{A-42}$$

where

$$
\begin{aligned}
k &= \text{von Karman constant, } \textit{0.4} \\
l &= \text{vertical length scale taken as } \Delta z, \; \textit{m} \\
R_i &= \text{local Richardson number} \\
C &= \text{constant, } \textit{taken as 1.5}
\end{aligned}
$$

In the longitudinal-vertical model, the lateral velocity, V, and its gradient, $\partial V/\partial z$, are due to the lateral component of wind wave motion and are assumed to be zero when averaged laterally, but not necessarily the square $(\partial V/\partial z)^2$. It is assumed that cross wind shear τ_{wy} generates lateral wave components v'' such that $<w''v''> = \tau_{wy} e^{-2kz}$. Further, let

$$A_z^2 \left[\frac{\partial V}{\partial z} \right]^2 = \left[\tau_{wy} e^{-2kz} \right]^2 \tag{A-43}$$

giving for cross wind shear:

$$\left[\frac{\partial V}{\partial z} \right]^2 = \left[\frac{\tau_{wy} e^{-2kz}}{A_z} \right]^2 \tag{A-44}$$

Thus, eddy viscosity with cross wind shear becomes:

$$A_z = k \left[\frac{l^2}{2} \right] \sqrt{ \left[\frac{\partial U}{\partial z} \right]^2 + \left[\frac{\tau_{wy} e^{-2kz}}{A_z} \right]^2 } \ e^{(-CR_i)} \qquad (A\text{-}45)$$

In numerical form, A_z can be iterated from equation (A-45) by using a value at the previous timestep to evaluate cross wind shear contribution. A_z should not be less than the molecular kinematic viscosity for water. For the present hydrodynamic solution, there is also the limit that $A_z < \Delta z^2/\Delta t$. Version 3.0 will eliminate this restriction.

The above formulation of wind shear in horizontal momentum and evaluation of A_z leads to wind driven surface currents that are three to ten percent of the surface wind velocity with higher values appearing at higher wind speeds. This is in accordance with the few attempts to relate wind speed and surface current velocity from field data appearing in the literature. With the formulation, the surface current does not reach abnormal values as it does for the case of wind shear applied only to the surface and as the surface layer thickness decreases. The depth of the wind driven surface layer increases with wind speed, and mass transport due to wind appears to be insensitive to the finite difference layer thickness.

The wind wave formulation is based on the significant wave height and period. There is a whole spectrum of wind wave components, u'' and v'', equations (A-39) and (A-40), and hence a whole spectrum of wind wave decay rates producing a spectrum of wind shears. It is presently not known if the major portion of the wind shear is propagated by waves making up the significant wave height and period portion of the wind wave spectrum. The present formulation provides the basis for further theoretical investigations. A k-ϵ turbulence model is presently undergoing testing and may be included as an option in Version 3.0.

Heat Budget

Surface Heat Exchange. Surface heat exchange can be formulated as a term-by-term process using the explicit adjacent cell transport computation as long as the integration timestep is shorter than or equal to the frequency of the meteorological data. Surface heat exchange processes depending on water surface temperatures are computed using previous timestep data and are therefore lagged from transport processes by the integration timestep.

Term-by-term surface heat exchange is computed as:

$$H_n = H_s + H_a + H_e + H_c - (H_{sr} + H_{ar} + H_{br}) \qquad \text{(A-46)}$$

where

H_n = the net rate of heat exchange across the water surface, $W\,m^{-2}$
H_s = incident short wave solar radiation, $W\,m^{-2}$
H_a = incident long wave radiation, $W\,m^{-2}$
H_{sr} = reflected short wave solar radiation, $W\,m^{-2}$
H_{ar} = reflected long wave radiation, $W\,m^{-2}$
H_{br} = back radiation from the water surface, $W\,m^{-2}$
H_e = evaporative heat loss, $W\,m^{-2}$
H_c = heat conduction, $W\,m^{-2}$

The short wave solar radiation is either measured directly or computed from sun angle relationships and cloud cover. The long wave atmospheric radiation is computed from air temperature and cloud cover or air vapor pressure using Brunts formula. The right-hand terms are all water surface temperature dependent.

Water surface back radiation is computed as:

$$H_{br} = \varepsilon \sigma^* (T_s + 273.15)^4 \qquad \text{(A-47)}$$

where

ε = emissivity of water, *0.97*
σ^* = Stephan-Boltzman constant, *5.67 x 10^{-8} W m^{-2} °K^{-4}*
T_s = water surface temperature, *°C*

Like the remaining terms, it is computed for each surface layer cell on each iteration timestep.

Evaporative heat loss is computed as:

$$H_e = f(W)\,(e_s - e_a) \qquad \text{(A-48)}$$

where

$f(W)$ = evaporative wind speed function, *W m^{-2} mm Hg^{-1}*
e_s = saturation vapor pressure at the water surface, *mm Hg*
e_a = atmospheric vapor pressure, *mm Hg*

Evaporative heat loss depends on air temperature and dew point temperature or relative humidity. Surface vapor pressure is computed from the surface temperature for each surface cell on each iteration.

Surface heat conduction is computed as:

$$H_c = C_c \, f(W) \, (T_s - T_a) \qquad \text{(A-49)}$$

where

C_c = Bowen's coefficient, *0.47 mm Hg $°C^1$*

T_a = air temperature, $°C$

Short wave solar radiation penetrates the surface and decays exponentially with depth according to Bears Law:

$$H_s(z) = (1 - \beta) \, H_s \, e^{-\eta z} \qquad \text{(A-50)}$$

where

$H_s(z)$ = short wave radiation at depth z, $W \, m^{-2}$

β = fraction absorbed at the water surface

η = extinction coefficient, m^{-1}

H_s = short wave radiation reaching the surface, $W \, m^{-2}$

Aside from the problems of measuring meteorological data relative to a large waterbody and especially the problem of translating climatological data from distant weather stations, the most uncertain parameter in the surface heat exchange computations is the evaporative wind speed function, f(W). Various formulations of f(W) have been catalogued and examined in Edinger, et al. (1974). Unlike the use of wind speed in wind shear relations as discussed in the previous section, evaporative wind speed is thought to be a "ventilation speed" rather than a vector velocity. The different formulations result from the empirical determination of f(W) for different size and shape waterbodies with data from different locations and averaged over different periods of time.

Since certain of the terms in equation (A-46) are surface temperature dependent, and others are measurable or computable input variables, the most direct route is to define an equilibrium temperature, T_e, as the temperature at which the net rate of surface heat exchange is zero. Equilibrium temperature is the fictitious water surface temperature at which incoming radiation heat rates are just balanced by outgoing water surface temperature dependent processes.

Linearization of equation (A-46) along with the definition of equilibrium temperature allows expressing the net rate of surface heat exchange, H_n, as:

$$H_n = -K_{aw}(T_w - T_e)$$ (A-51)

where

H_n = rate of surface heat exchange, W m^{-2}
K_{aw} = coefficient of surface heat exchange, $W\ m^{-2}\ °C^{-1}$
T_w = water surface temperature, $°C$
T_e = equilibrium temperature, $°C$

Seven separate heat exchange processes are summarized in the coefficient of surface heat exchange and equilibrium temperature. The linearization used in obtaining equation (A-51) has been examined in detail by Brady, et al. (1968), and Edinger et al. (1974).

The definition of the coefficient of surface heat exchange can be shown to be the first term of a Taylor series expansion by considering equation (A-51) as:

$$H_n = -\frac{dH_n}{dT_s}(T_s - T_e)$$ (A-52)

where the derivative of H_n with respect to surface temperature is evaluated from equation (A-46) to give K_{aw}, the coefficient of surface heat exchange. All approximations of the individual surface heat exchange terms enter into the evaluation of the coefficient of surface heat exchange and the equilibrium temperature. Equations (A-47) and (A-48) are defined from equation (A-46). They have the same difficulties in evaluation as the individual terms in equation (A-46), but provide a simpler algebraic method for including surface heat exchange in temperature analyses.

The mass evaporation rate is computed by dividing evaporative heat loss by the latent heat of evaporation of water. Surface heat exchange *always* includes evaporative heat loss in the heat budget, but the user may choose to exclude it in the water budget. For many reservoirs, inflow rates are determined from storage estimates that implicitly include evaporation.

Sediment Heat Exchange. Sediment heat exchange with water is generally small compared to surface heat exchange and many previous modelers have neglected it. Version 2.0 of the model now includes sediment/water heat exchange. Investigations on several reservoirs have shown the process must be included to accurately reproduce hypolimnetic temperatures primarily because

of the reduction in numerical diffusion. The formulation is similar to surface heat exchange:

$$H_{sw} = -K_{sw}(T_w - T_s)$$ (A-53)

where

H_{sw} = rate of sediment/water heat exchange, $W\ m^{-2}$
K_{sw} = coefficient of sediment/water heat exchange, $W\ m^{-2}\ {}^{\circ}C^{-1}$
T_w = water temperature, ${}^{\circ}C$
T_s = sediment temperature, ${}^{\circ}C$

Previous applications used a value of $7 \times 10^{-8}\ W\ m^{-2}\ {}^{\circ}C^{-1}$ for K_{sw} which is approximately 2 orders of magnitude smaller than the surface heat exchange coefficient. Average yearly air temperature is a good estimate of T_s.

Ice Cover

Ice thickness and onset and loss of ice cover play an important role in the heat budget of northern waterbodies. At high latitudes, ice cover may remain until late spring or early summer and prevent warming due to absorption of short wave solar radiation.

The ice model is based on an ice cover with ice-to-air heat exchange, conduction through the ice, conduction between underlying water, and a "melt temperature" layer on the ice bottom (Ashton, 1979). The overall heat balance for the water-to-ice-to-air system is:

$$\rho_i\ L_f\ \frac{\Delta h}{\Delta t} = h_{ai}(T_i - T_e) - h_{wi}(T_w - T_m)$$ (A-54)

where

ρ_i = density of ice, $kg\ m^{-3}$
L_f = latent heat of fusion of ice, $J\ kg^{-1}$
$\Delta h/\Delta t$ = change in ice thickness (h) with time (t), $m\ sec^{-1}$
h_{ai} = coefficient of ice-to-air heat exchange, $W\ m^{-2}\ {}^{\circ}C^{-1}$
h_{wi} = coefficient of water-to-ice heat exchange through the melt layer, $W\ m^{-2}\ {}^{\circ}C^{-1}$
T_i = ice temperature, ${}^{\circ}C$
T_{ei} = equilibrium temperature of ice-to-air heat exchange, ${}^{\circ}C$
T_w = water temperature below ice, ${}^{\circ}C$
T_m = melt temperature, $0{}^{\circ}C$

The ice-to-air coefficient of surface heat exchange, h_{ai}, and its equilibrium temperature, T_{ei}, are computed the same as for surface heat exchange in Edin-

ger, et al. (1974) because heat balance of the thin, ice surface water layer is the same as the net rate of surface heat exchange presented previously. The coefficient of water-to-ice exchange, h_{wi}, depends on turbulence and water movement under ice and their effect on melt layer thickness. It is a function of water velocity for rivers but must be empirically adjusted for reservoirs.

Ice temperature in the ice-heat balance is computed by equating the rate of surface heat transfer between ice and air to the rate of heat conduction through ice:

$$h_{ai}(T_i - T_{ei}) = \frac{-k_i(T_i - T_m)}{h} \qquad \text{(A-55)}$$

where

k_i = molecular heat conductivity of ice, $W\,m^{-1}\,{}^{\circ}C^{-1}$

When solved for ice temperature, T_i, and inserted in the overall ice-heat balance, the ice thickness relationship becomes:

$$\frac{\rho_i L_f \Delta h}{\Delta t} = \frac{(T_M - T_{ei})}{\dfrac{h}{k_i} + \dfrac{1}{h_{ia}}} - h_{wi}(T_w - T_m) \qquad \text{(A-56)}$$

from which ice thickness can be computed for each longitudinal segment. Heat from water to ice transferred by the last term is removed in the water temperature transport computations.

Variations in the onset of ice cover and seasonal growth and melt over the waterbody depend on locations and temperatures of inflows and outflows, evaporative wind variations over the ice surface, and effects of water movement on the ice-to-water exchange coefficient. Ice will often form in reservoir branches before forming in the main pool and remain longer due to these effects.

A second, more detailed algorithm for computing ice growth and decay has been developed for the model. The algorithm consists of a series of one-dimensional, quasi steady-state, thermodynamic calculations for each timestep. It is similar to those of Maykut and Untersteiner (1971), Wake (1977) and Patterson and Hamblin (1988). The detailed algorithm provides a more accurate representation of the upper part of the ice temperature profile resulting in a more accurate calculation of ice surface temperature and rate of ice freezing and melting.

The ice surface temperature, T_s, is iteratively computed at each timestep using the upper boundary condition as follows. Assuming linear thermal gradients and using finite difference approximations, heat fluxes through the ice, q_i, and at the ice-water interface, q_{iw}, are computed. Ice thickness at time t, $\theta(t)$, is determined by ice melt at the air-ice interface, $\Delta\theta_{ai}$, and ice growth and melt at the ice-water interface, $\Delta\theta_{iw}$. The computational sequence of ice cover is presented below.

Initial ice formation. Formation of ice requires lowering the surface water temperature to the freezing point by normal surface heat exchange processes. With further heat removal, ice begins to form on the water surface. This is indicated by a negative water surface temperature. The negative water surface temperature is then converted to equivalent ice thickness and equivalent heat is added to the heat source and sink term for water. The computation is done once for each segment beginning with the ice-free period:

$$\theta_0 = \frac{-T_{w_n}\rho_w C_{P_w} h}{\rho_i L_f} \tag{A-57}$$

where

θ_0 = thickness of initial ice formation during a timestep, *m*
T_{w_n} = local temporary negative water temperature, *°C*
h = layer thickness, *m*
ρ_w = density of water, *kg m^{-3}*
C_{P_w} = specific heat of water, *J kg^{-1} °C^{-1}*
ρ_i = density of ice, *kg m^{-3}*
L_f = latent heat of fusion, *J kg^{-1}*

Upper air-ice interface flux boundary condition and ice surface temperature approximation: The ice surface temperature, T_s, must be known to calculate the heat components, H_{br}, H_e, H_c, and the thermal gradient in the ice since the components and gradient all are either explicitly or implicitly a function of T_s. Except during the active thawing season when ice surface temperature is constant at 0 °C, T_s must be computed at each timestep using the upper boundary condition. The approximate value for T_s is obtained by linearizing the ice thickness across the timestep and solving for T_s.

$$q_i = K_i \frac{T_f - T_s(t)}{\theta(t)} \tag{A-58}$$

$$H_{sn} + H_{an} - H_{br} - H_e - H_c + q_i = \rho_i L_f \frac{d\theta_{ai}}{dt}, \quad \text{for } T_s = 0°C \tag{A-59}$$

$$T_s^n \approx \frac{\theta^{n-1}}{K_i}\left[H_{sn}^n + H_{an}^n - H_{br}T_s^n - H_eT_s^n - H_cT_s^n\right] \qquad (A\text{-}60)$$

where

K_i = thermal conductivity of ice, $W\,m^{-1}\,{}^{\circ}C^{-1}$

T_f = freezing point temperature, ${}^{\circ}C$

n = time level

Absorbed solar radiation by the water under the ice. Although the amount of penetrated solar radiation is relatively small, it is an important component of the heat budget since it is the only heat source to the water column when ice is present and may contribute significantly to ice melting at the ice-water interface. The amount of solar radiation absorbed by water under the ice cover may be expressed as:

$$H_{ps} = H_s(1-ALB_i)(1-\beta_i)\,e^{-\gamma_i\,\theta(t)} \qquad (A\text{-}61)$$

where

H_{ps} = solar radiation absorbed by water under ice cover, $W\,m^{-2}$

H_s = incident solar radiation, $W\,m^{-2}$

ALB_i = ice albedo

β_i = fraction of the incoming solar radiation absorbed in the ice surface

γ_i = ice extinction coefficient, m^{-1}

Ice melt at the air-ice interface. The solution for T_s holds as long as net surface heat exchange, $H_n(T_s)$, remains negative corresponding to surface cooling, and surface melting cannot occur. If $H_n(T_s)$ becomes positive corresponding to a net gain of heat at the surface, q_i must become negative and an equilibrium solution can only exist if $T_s > T_f$. This situation is not possible as melting will occur at the surface before equilibrium is reached (Patterson and Hamblin, 1988). As a result of quasi-steady approximation, heat, which in reality is used to melt ice at the surface, is stored internally producing an unrealistic temperature profile. Stored energy is used for melting at each timestep and since total energy input is the same, net error is small. Stored energy used for melting ice is expressed as:

$$\rho_i\,C_{p_i}\frac{T_s(t)}{2}\,\theta(t) = \rho_i L_f \Delta\theta_{ai} \qquad (A\text{-}62)$$

where

C_{pi} = specific heat of ice, $J\,kg^{-1}\,{}^{\circ}C^{-1}$

θ_{ai} = ice melt at the air-ice interface, m^{-1}

Formulation of lower ice-water interface flux boundary condition. Both ice growth and melt may occur at the ice-water interface. The interface temperature, T_f, is fixed by the water properties. Flux of heat in the ice at the interface therefore depends on T_f and the surface temperature T_s through the heat flux q_i. Independently, heat flux from the water to ice, q_{iw}, depends only on conditions beneath the ice. An imbalance between these fluxes provides a mechanism for freezing or melting. Thus,

$$q_i - q_{iw} = \rho_i L_f \frac{d\theta_{iw}}{dt} \qquad \text{(A-63)}$$

where

θ_{iw} = ice growth/melt at the ice-water interface

The coefficient of water-to-ice exchange, K_{wi}, depends on turbulence and water movement under the ice and their effect on melt layer thickness. It is known to be a function of water velocity for rivers and streams but must be empirically adjusted for reservoirs. The heat flux at the ice-water interface is:

$$q_{iw} = h_{wi}\left(T_w(t) - T_f\right) \qquad \text{(A-64)}$$

where

T_w = water temperature in the uppermost layer under the ice, $^{\circ}C$

Finally, ice growth or melt at the ice-water interface is:

$$\Delta\theta_{iw}^n = \frac{1}{\rho_i L_f}\left[K_i \frac{T_f - T_s^n}{\theta^{n-1}} - h_{wi}(T_w^n - T_f)\right] \qquad \text{(A-65)}$$

Density

Accurate hydrodynamic calculations require accurate water densities. Water densities are affected by variations in temperature and solids concentrations given by :

$$\rho = \rho_T + \Delta\rho_S \qquad \text{(A-66)}$$

where

ρ = density, $kg\ m^{-3}$
ρ_T = water density as a function of temperature, $kg\ m^{-3}$
$\Delta\rho_S$ = density increment due to solids, $kg\ m^{-3}$

A variety of formulations have been proposed to describe water density variations due to temperatures. The following relationship is used in the model (Gill, 1982):

$$\rho_{T_w} = 999.8452594 + 6.793952 \times 10^{-2} \ T_w$$
$$- 9.095290 \times 10^{-3} \ T_w^2 + 1.001685 \times 10^{-4} \ T_w^3 \qquad \text{(A-67)}$$
$$- 1.120083 \times 10^{-6} \ T_w^4 + 6.536332 \times 10^{-9} \times T_w^5$$

Suspended and dissolved solids also affect density. For most applications, dissolved solids will be in the form of total dissolved solids (TDS). For estuarine applications, salinity should be specified. The effect of dissolved solids on density is calculated using either of these variables with the choice specified by the variable [WTYPE] (see page C11). Density effects due to TDS are given by Ford and Johnson (1983):

$$\Delta\rho_{TDS} = (8.221 \times 10^{-4} - 3.87 \times 10^{-6} \ T_w + 4.99 \times 10^{-8} \ T_w^2) \ \Phi_{TDS} \qquad \text{(A-68)}$$

where

$$\Phi_{TDS} \quad = \text{TDS concentration, } g \ m^{-3}$$

and for salinity (Gill, 1982):

$$\Delta\rho_{sal} = (0.824493 - 4.0899 \times 10^{-3} \ T_w + 7.6438 \times 10^{-5} \ T_w^2$$
$$- 8.2467 \times 10^{-7} \ T_w^3 + 5.3875 \times 10^{-9} \ T_w^4) \ \Phi_{sal}$$
$$+ (-5.72466 \times 10^{-3} + 1.0227 \times 10^{-4} \ T_w \qquad \text{(A-69)}$$
$$- 1.6546 \times 10^{-6} \ T_w^2) \ \Phi_{sal}^{1.5} + 4.8314 \times 10^{-4} \ \Phi_{sal}^2$$

where

$$\Phi_{sal} = \text{salinity, } kg \ m^{-3}$$

The suspended solids effects are given by Ford and Johnson (1983):

$$\Delta\rho_{ss} = \Phi_{ss} \left[1 - \frac{1}{SG} \right] \times 10^{-3} \qquad \text{(A-70)}$$

where

Φ_{ss} = suspended solids concentration, $g\ m^{-3}$
SG = specific gravity of suspended solids

Assuming a specific gravity of 2.65, the above relationship is simplified to:

$$\Delta\rho_{ss} = 0.00062\ \Phi_{ss} \qquad \text{(A-71)}$$

The total effect of solids is then:

$$\Delta\rho_{s} = (\Delta\rho_{sal}\ \text{or}\ \Delta\rho_{tds}) + \Delta\rho_{ss} \qquad \text{(A-72)}$$

Selective Withdrawal

Outflows from reservoirs are usually from outlets on the order of a model layer in thickness. The code provides an option to either specify flows from particular layers at downstream segments or a selective withdrawal algorithm where outflows and layer locations are calculated based on the total outflow [QOUT], structure type [SINK] and elevation [ELSTR], and computed upstream density gradients. The selective withdrawal computation uses these values to compute vertical withdrawal zone limits and outflows. It also sums the outflows for multiple structures.

Outflow distribution is calculated in the subroutine SELECTIVE_WITH-DRAWAL. This routine first calculates limits of withdrawal based on either a user specified point or line sink approximation for outlet geometry [SINK]. The empirical expression for point sink withdrawal limits is:

$$d = (c_{bi}Q/N)^{0.3333} \qquad \text{(A-73)}$$

and for a line sink:

$$d = (c_{bi}2q/N)^{0.5} \qquad \text{(A-74)}$$

where

d = withdrawal zone half height, m
Q = total outflow, $m^{3}\ s^{-1}$
N = internal buoyancy frequency, Hz
q = outflow per unit width, $m^{2}\ s^{-1}$
c_{bi} = boundary interference coefficient

The width is the outlet width. The point sink approximation assumes approach flow is radial both longitudinally and vertically while the line sink approximation assumes flow approaches the outlet radially in the vertical. The boundary interference coefficient is two near a physical boundary and one elsewhere.

Velocities are determined using a quadratic shape function:

$$V_k = 1 - \left[\frac{(\rho_k - \rho_o)}{(\rho_1 - \rho_o)} \right]^2 \qquad \text{(A-75)}$$

where

V_k = normalized velocity in layer k
ρ_k = density in layer k, $kg\ m^{-3}$
ρ_o = density in the outlet layer, $kg\ m^{-3}$
ρ_1 = density of the withdrawal limit layer, $kg\ m^{-3}$

The shape function generates a maximum velocity at the outlet level with velocities approaching zero at withdrawal limits. During non-stratified periods, outflow from top to bottom is uniform. Uniform flows also result from large outflows during periods of mild stratification. As stratification develops, withdrawal limits decrease and outflow is weighted towards the outlet elevation.

Withdrawal limits can be varied by specifying a line sink and changing the effective width. Small outlet widths result in nearly uniform outflows, while large widths limit outflows to the outlet layer.

Appendix B
Water Quality

The constituent transport relationships described in Appendix A compute the transport of constituents with their kinetic reaction rates expressed in source and sink terms. All sources/sinks (both internal and external) for water temperature are contained in the array [TSS]. The sources/sinks for constituents are separated into two arrays, [CSSB] and [CSSK]. [CSSB] contains boundary sources/sinks. [CSSK] contains internal sources/sinks due to kinetic reactions. The reactions are computed in subroutines for all nonconservative materials. The division of terms allows kinetic sources/sinks to be updated at different frequencies than boundary sources/sinks - consistent with coarser time scales associated with biological and chemical processes as opposed to hydrodynamics. Computational time is also reduced. The frequency at which kinetic sources/sinks [CSSK] are updated is specified by the parameter [FREQUK] (see page C69).

The source/sink term [CSSK] represents a mass rate of change (grams per second) of a constituent due to kinetic reactions where concentrations are expressed as grams per meter^3. The kinetic reactions can be depicted graphically by considering each constituent as a compartment. Mass transfer rates between compartments are represented by arrows, with a source represented by an arrow leading to the compartment and a sink by an arrow leading away. The rate equation for a particular constituent can be developed directly from the graphical representation. Both graphical and mathematical descriptions of the rate equation for each constituent are provided.

All rate terms used in the equations are in units of per second. These rates are converted internally from units of per day specified in the control file (see Appendix C).

Conservative Tracer

A conservative constituent is included to allow dye study simulations, movements of conservative materials through the waterbody, and as an aid in calibrating and testing flow regimes. As a conservative material, this constituent has no internal sources or sinks and the rate term [CSSK] is set to zero.

Inorganic Suspended Solids

Inorganic suspended solids are important in water quality simulations because of their influence on density, light penetration, and nutrient availability. Increased solids concentrations reduce light penetration in the water column thus affecting temperature which in turn affects biological and chemical reaction rates. Nutrient concentrations are also affected by solids through adsorption and settling. Light and nutrient availability largely control algal production.
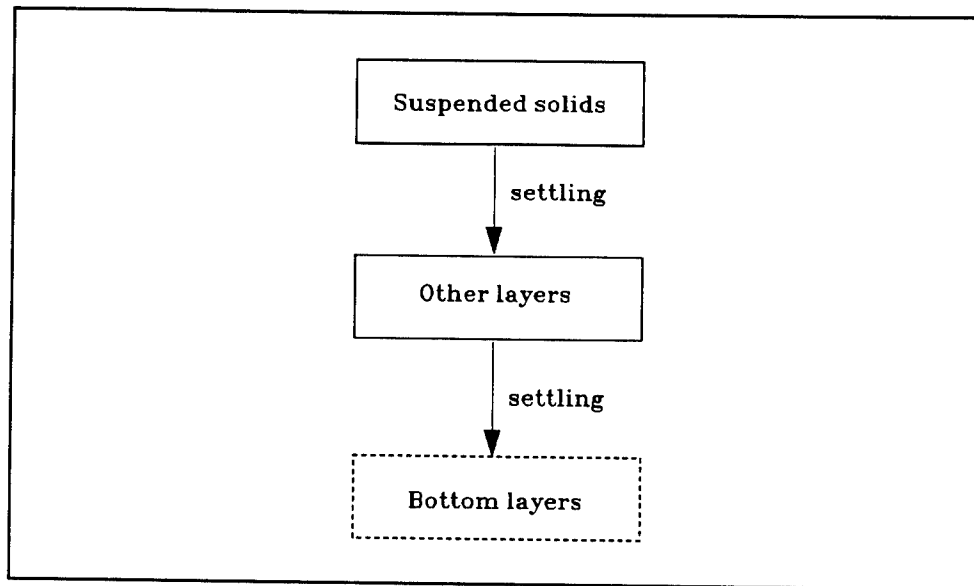
Figure B-1. Internal flux for inorganic suspended solids.

Referring to Figure B-1, the rate equation for inorganic suspended solids is:

$$\frac{\partial \Phi_{ss}}{\partial t} = -\frac{\omega_{ss}}{\Delta z} \Phi_{ss} \qquad \text{(B-1)}$$

where

ω_{ss} = settling velocity, $m\ sec^{-1}$
Φ_{ss} = suspended solids concentration, $g\ m^{-3}$
Δz = cell thickness, m

In the finite difference representation of suspended solids concentrations, solids settling from layer [K]-1 serve as a source for the layer below it [K]. No provision is made to accumulate inorganic solids or allow resuspension in the sediments. Version 3.0 of the model will include these processes in a sediment

transport compartment. Lateral averaging results in homogeneous solids concentrations laterally. In reality, concentrations generally decrease with distance away from the dominant flow path. This effect is not included. The rate term for inorganic suspended solids is evaluated in the subroutine SUSPENDED_SOLIDS.

Coliform Bacteria

Coliform bacteria is commonly used as an indicator of pathogen contamination. Safety standards and criteria for drinking and recreational purposes are based upon coliform concentrations. Predictions of coliform bacteria are important because of their impact on recreation and water supply.
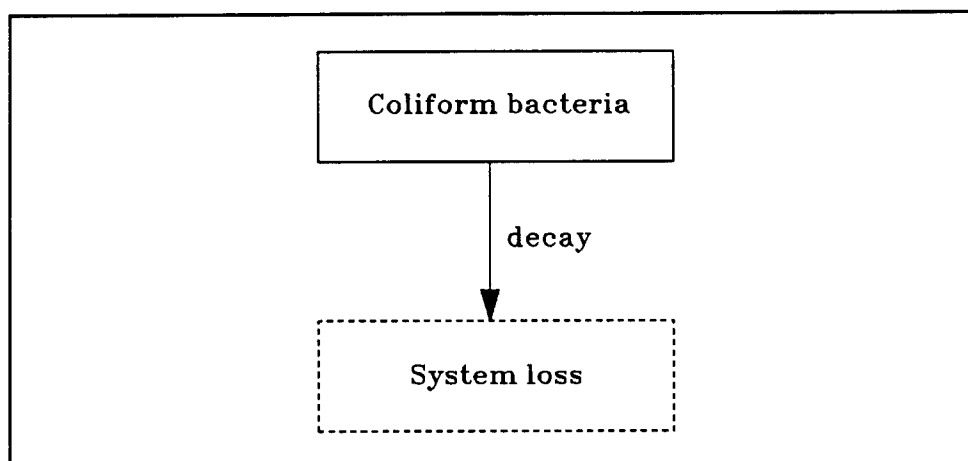
Figure B-2. Internal flux for coliform bacteria.

Total coliforms, fecal coliforms, or fecal streptococci are simulated with this compartment and are independent of all other compartments except temperature. Referring to Figure B-2, the rate equation for coliforms is:

$$\frac{\partial \Phi_{col}}{\partial t} = -K_{col} \, \theta^{(T-20)} \, \Phi_{col} \qquad \text{(B-2)}$$

where

K_{col} = coliform mortality, sec^{-1}
θ = temperature factor (Q10)
T = water temperature, $°C$
Φ_{col} = coliform concentration, $g \ m^{-3}$

and the rate term is evaluated in the subroutine COLIFORM.

The Q10 formulation arises from a doubling of the reaction rate with each $10\,^\circ C$ increase in temperature. This doubling rate has not been found at lower temperatures (Hargrave 1972b) and is quite variable for various reactions (Giese 1968). Modeling coliform bacteria is discussed in detail in Zison, et al. (1978).

Total Dissolved Solids or Salinity

Total dissolved solids (TDS) effect both water density and ionic strength, thereby affecting water movements, pH, and the distribution of carbonate species. Dissolved solids are normally expressed as total dissolved solids (TDS) in freshwater applications. Estuarine applications normally use salinity. Either TDS or salinity can be used with the choice indicated by the parameter [WTYPE] specified in the control file (see page C11). The choice is then reflected in the computation of density and ionic strength. If TDS is used, the units are grams per meter^3, while salinity is kilograms per meter^3. It is important to keep in mind TDS and salinity are not equivalent - salinity is conservative while TDS is not. In the model, however, both are treated conservatively with the rate term set to zero.

Labile DOM

Because of the importance of dissolved oxygen in aquatic systems, all constituents exerting an oxygen demand must be included in kinetic formulations. This demand is often measured in rivers as the biochemical oxygen demand (BOD), which includes microbial respiration and metabolism of various organic and inorganic compounds. However, production of these materials occurs as well as decomposition, requiring the major components of BOD be modeled individually. One of these constituents is dissolved organic matter (DOM), which is composed of labile and refractory components. DOM is modeled as two separate compartments because of the two groups' different decomposition rates.

Referring to Figure B-3, the rate equation for labile DOM is:

$$\partial \Phi_{ldom} = K_{ac}\Phi_a + (1 - P_{am})K_{am}\Phi_a - \gamma_{om}K_{ldom}\Phi_{ldom} - K_{l \to r}\Phi_{ldom} \qquad \text{(B-3)}$$

where

K_{ac} = algal excretion rate, sec^{-1} (see equation B-12)
K_{am} = algal mortality rate, sec^{-1} (see equation B-13)
K_{ldom} = labile DOM decay rate, sec^{-1}
$K_{l \to r}$ = transfer rate from labile to refractory DOM, sec^{-1}
P_{am} = pattern coefficient for algal mortality
γ_{om} = temperature rate multiplier for organic matter decay
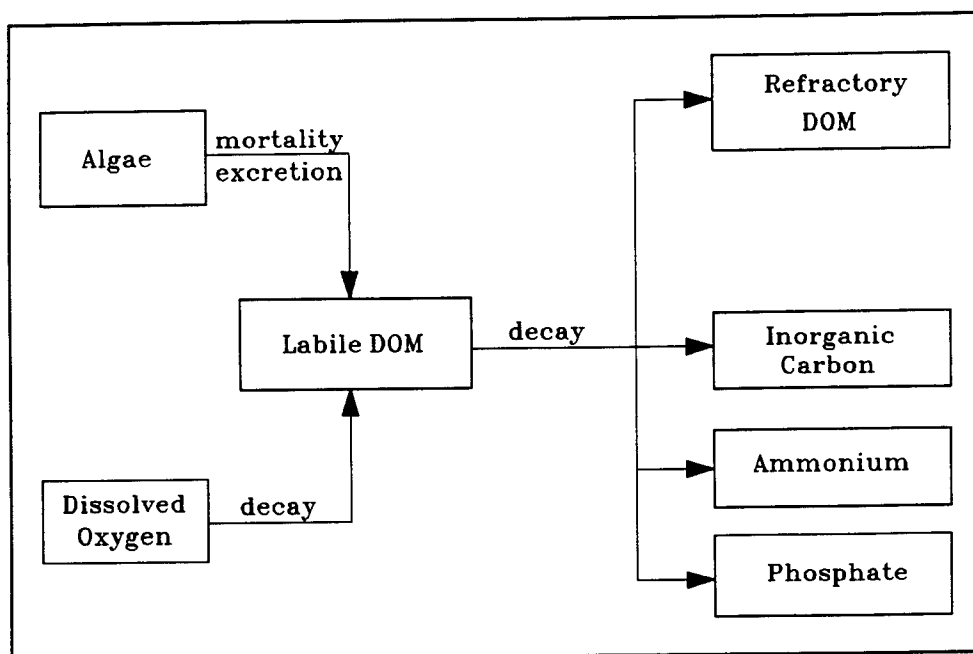
Figure B-3. Internal flux between labile DOM and other compartments

Φ_a = algal concentration, $g\ m^{-3}$

Φ_{ldom} = labile DOM concentration, $g\ m^{-3}$

and the rate terms are evaluated in subroutine LABILE_DOM. Where applications only require simulation of dissolved oxygen and BOD, this compartment would be turned off and BOD would be included in the simulation. If organic loading rates are available as BOD and algal/nutrient interactions are modeled, then both compartments would be included in the simulation.

Refractory DOM

Refractory DOM is composed of compounds in the aquatic environment that slowly decompose exerting oxygen demand over long periods. Internally, refractory DOM is produced from the decomposition of labile DOM.
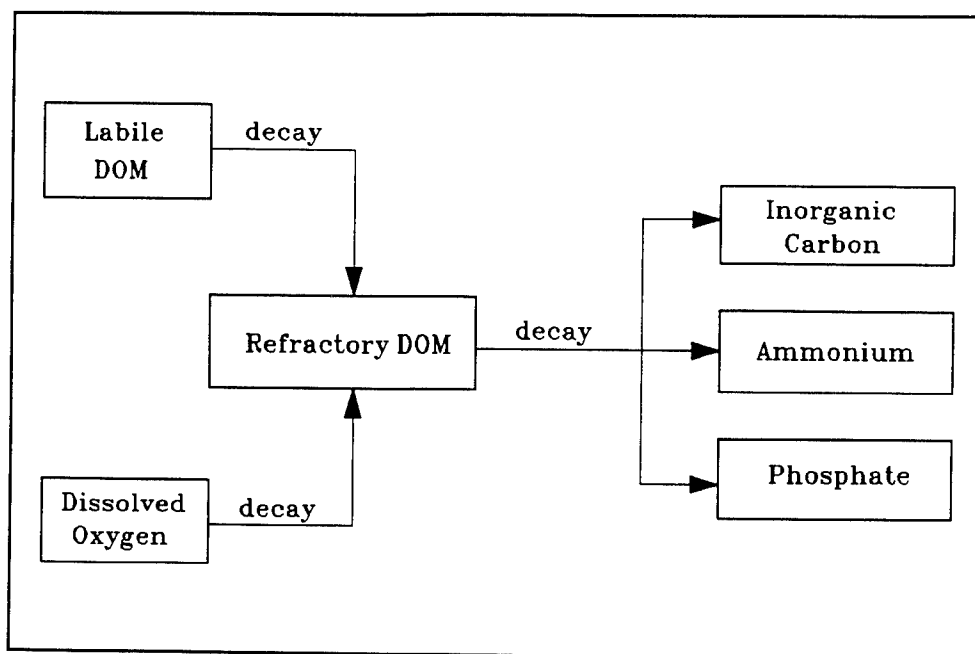
Figure B-4. Internal flux between refractory DOM and other compartments.

Referring to Figure B-4, the rate equation for refractory DOM is:

$$\frac{\partial \Phi_{rdom}}{\partial t} = K_{l\rightarrow r}\Phi_{ldom} - \gamma_{om}K_{rdom}\Phi_{rdom} \qquad \text{(B-4)}$$

where

$K_{l\rightarrow r}$ = transfer rate from labile DOM, sec^{-1}

C_{ldom} = concentration of labile DOM, $g\ m^{-3}$

γ_{om} = temperature rate multiplier

K_{rdom} = refractory DOM decay rate, sec^{-1}

Φ_{rdom} = refractory DOM concentration, $g\ m^{-3}$

and the rate terms are evaluated in subroutine REFRACTORY_DOM.

Detritus

Detritus represents particulate organic material in the water column. When decaying, detritus is a source of nitrogen, phosphorus, and carbon. A stoichiometric relationship is used to release ammonium-nitrogen, phosphorus, and carbon, and an oxygen demand is exerted as detritus decomposes. When detritus settles to the bottom, it accumulates and decays in the sediment compartment if the sediment compartment is included in the simulation (see page C71).
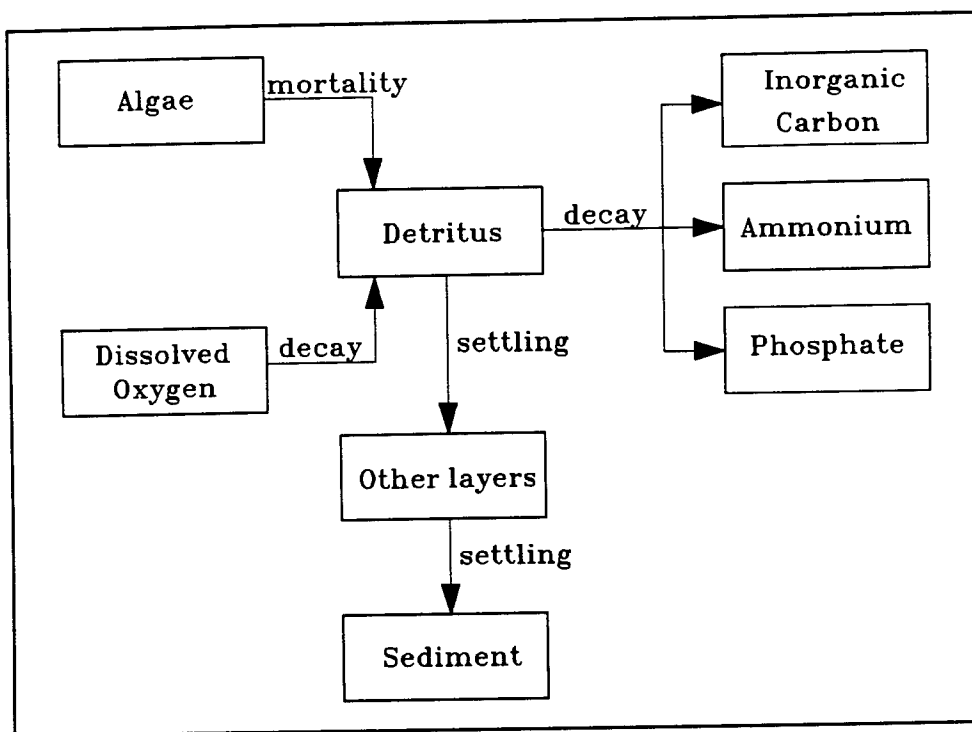
Figure B-5. Internal flux between detritus and other compartments.

Referring to Figure B-4, the rate equation for detritus is:

$$\frac{\partial \Phi_{dt}}{\partial t} = P_{am}K_{am}\Phi_a - K_{dt}\gamma_{om}\Phi_{dt} - \frac{\omega_{dt}}{\Delta z}\Phi_{dt} \qquad \text{(B-14)}$$

where

P_{am} = partition coefficient for algal mortality
K_{am} = algal mortality rate, sec^{-1} (see equation B-13)
Φ_a = algal concentration, $g\ m^{-3}$
K_{dt} = detritus decay rate, sec^{-1}
ω_{dt} = detritus settling rate, $m\ sec^{-1}$
Φ_{dt} = detritus concentration, $g\ m^{-3}$
Δz = model cell thickness, m
γ_{om} = temperature rate multiplier for organic matter

and the rate terms are evaluated in subroutine DETRITUS. Detritus settling and accumulation in the sediment compartment is handled identically to the algal compartment.

Algae

CE-QUAL-W2 uses a single compartment to represent algae. This representation precludes modeling algal succession for diatoms, greens, and blue-greens. However, an algal compartment does allow simulating the interaction between nutrients, algae, and dissolved oxygen.
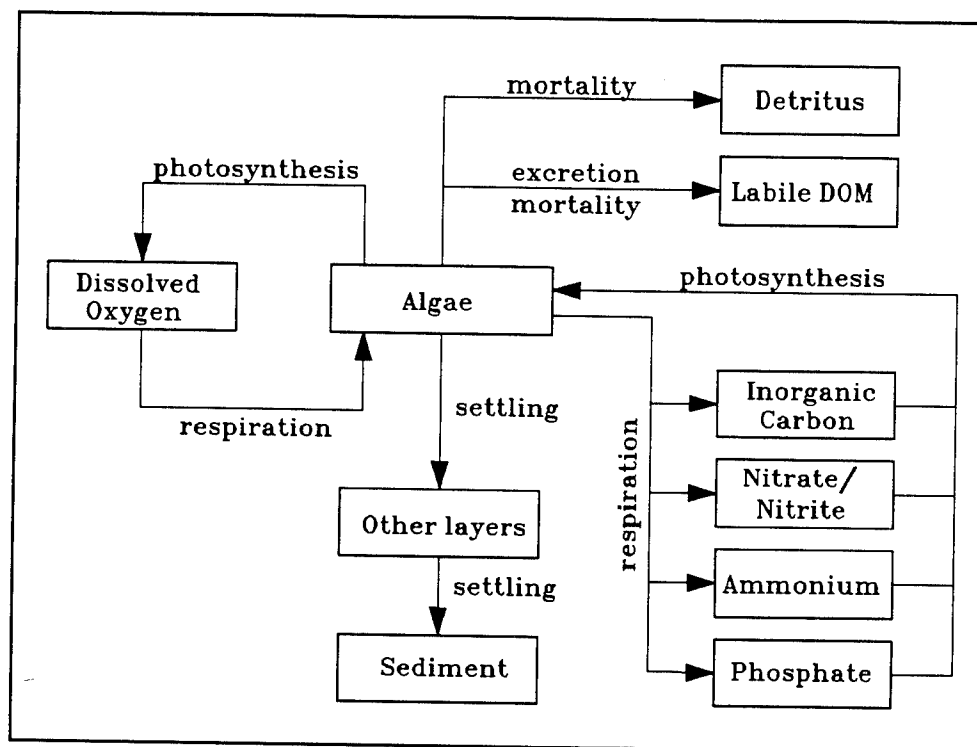
Figure B-6. Internal flux between algae and other compartments.

Referring to Figure B-6, the rate equation for algae is:

$$\frac{\partial \Phi_a}{\partial t} = K_{ag}\Phi_a - K_{ar}\Phi_a - K_{ae}\Phi_a - K_{am}\Phi_a - \frac{\omega_a}{\Delta z}\Phi_a \qquad \text{(B-5)}$$

where

Δz =   cell thickness, m

K_{ag} =   algal growth rate, sec^{-1} (see equation B-6)

K_{ar} =   algal dark respiration rate, sec^{-1} (see equation B-11)

K_{ae} =   algal excretion rate, sec^{-1} (see equation B-12)

K_{am} =   algal mortality rate, sec^{-1} (see equation B-13)

ω_a =   algal settling rate, $m\ sec^{-1}$

Φ_a = algal concentration, $g\ C\ m^{-3}$

and the rate terms are evaluated in subroutine PHYTOPLANKTON. Chlorophyl a is most commonly available as an estimate of algal biomass. To convert chlorophyll a to algal biomass, chlorophyll a is typically multiplied by 67. This value can vary widely depending on the makeup of the phytoplankton population. Some previous studies determined the conversion factor by regressing particulate organic matter with chlorophyll a.

Algal growth rate is computed by modifying a maximum growth rate affected by temperature, light, and nutrient availability:

$$K_{ag} = \gamma_{ar}\gamma_{af}\,\lambda_{min}K_{agmax} \qquad\qquad (B\text{-}6)$$

where

γ_{ar} = temperature rate multiplier for rising limb of curve
γ_{af} = temperature rate multiplier for falling limb of curve
λ_{min} = multiplier for limiting growth factor (minimum of light, phosphorus, and nitrogen)
K_{ag} = algal growth rate, sec^{-1}
K_{agmax} = maximum algal growth rate, sec^{-1}

Rate multipliers for algal growth are computed based upon available light (λ_l), phosphorus (λ_p), and nitrogen (λ_n). The rate multiplier for light is based upon the Steele (1962) function:

$$\lambda_l = \frac{I}{I_s}e^{\left(-\frac{I}{I_s}+1\right)} \qquad\qquad (B\text{-}7)$$

where

I = available light, $W\ m^{-2}$
I_s = saturating light intensity at maximum photosynthetic rate, $W\ m^{-2}$
λ_l = light limiting factor

The above expression allows for simulation of photoinhibition at light intensities greater than the saturation value. However, light penetration decreases with depth:

$$I = (1-\beta) I_0 e^{-\alpha z} \tag{B-8}$$

where

I_0 = solar radiation at the water surface, $W m^{-2}$
α = attenuation coefficient, m^{-2}
z = depth, m
β = fraction of solar radiation absorbed at the water surface

The average effect of light on algal growth in a particular model cell can be obtained by combining the above two expressions and integrating over the cell depth to obtain (Chapra and Reckhow, 1983):

$$\lambda_1 = \frac{e}{\alpha \Delta z} \left[e^{-\gamma_2} - e^{-\gamma_1} \right] \tag{B-9}$$

where

$$\gamma_1 = \frac{(1-\beta) I_0}{I_s} e^{-\alpha d}$$

$$\gamma_2 = \frac{(1-\beta) I_0}{I_s} e^{\alpha(d + \Delta z)}$$

d = depth at top of model cell, m

Units used for solar radiation in computing algal growth, Watts per square meter, differ from those used in heat exchange computations, degrees Celsius per meter per second. The model makes this conversion internally.

The fraction of solar radiation, βI_0, is added directly to the surface layer. The attenuation coefficient, α, consists of a baseline value [EXH2O] to which the effects of inorganic [EXINOR] and organic [EXORG] suspended solids are added (see page C79).

Rate multipliers limiting algal growth due to concentrations of phosphorus and nitrogen are computed using the Monod relationship:

$$\lambda_i = \frac{\Phi_i}{P_i + \Phi_i} \qquad \text{(B-10)}$$

where

Φ_i = phosphorus or nitrate + ammonia-nitrogen concentration, $g\ m^{-3}$

P_i = half-saturation coefficient for phosphorus or nitrate + ammonia-nitrogen, $g\ m^{-3}$

Algal dark respiration is computed using the rising limb of the temperature function:

$$K_{ar} = \gamma_{ar} K_{armax} \qquad \text{(B-11)}$$

where

K_{armax} = maximum dark respiration rate, sec^{-1}

Algal photorespiration (excretion) is evaluated using an inverse relation to the light rate multiplier:

$$K_{ae} = (1 - \lambda_l)\, K_{aemax} \qquad \text{(B-12)}$$

where

K_{aemax} = maximum excretion rate constant, sec^{-1}

λ_l = light limiting factor

Excretion rates increase at both low and high light intensities, with excretion products contributing to labile DOM.

Algal mortality is defined as:

$$K_{am} = \gamma_{ar} K_{ammax} \qquad \text{(B-13)}$$

where

K_{ammax} = maximum mortality rate, sec^{-1}

This mortality rate represents both natural and predator mortality. Algal growth does not occur in the absence of light. Algal growth is not allowed to

exceed the limit imposed by nutrient supply over a given timestep. Algal excretion is not allowed to exceed algal growth rates.

Similar to inorganic solids, settling algae serve as a source for the layer below. Unlike inorganic solids, algae passing to the sediments accumulate within the sediment compartment. Detritus is also accumulated.

Phosphorus

Phosphorus is an important element in aquatic ecosystems since it serves as one of the primary nutrients for phytoplankton growth. In many fresh waters, phosphorus is considered to be the nutrient limiting maximum production of phytoplankton biomass (Schindler, 1971; Schindler et al., 1973; Vollenweider, 1968, 1976).

Phosphorus is assumed to be completely available as orthophosphate (PO_4) for uptake by phytoplankton. Measurements of soluble reactive phosphorus are closest to the form used in the model.
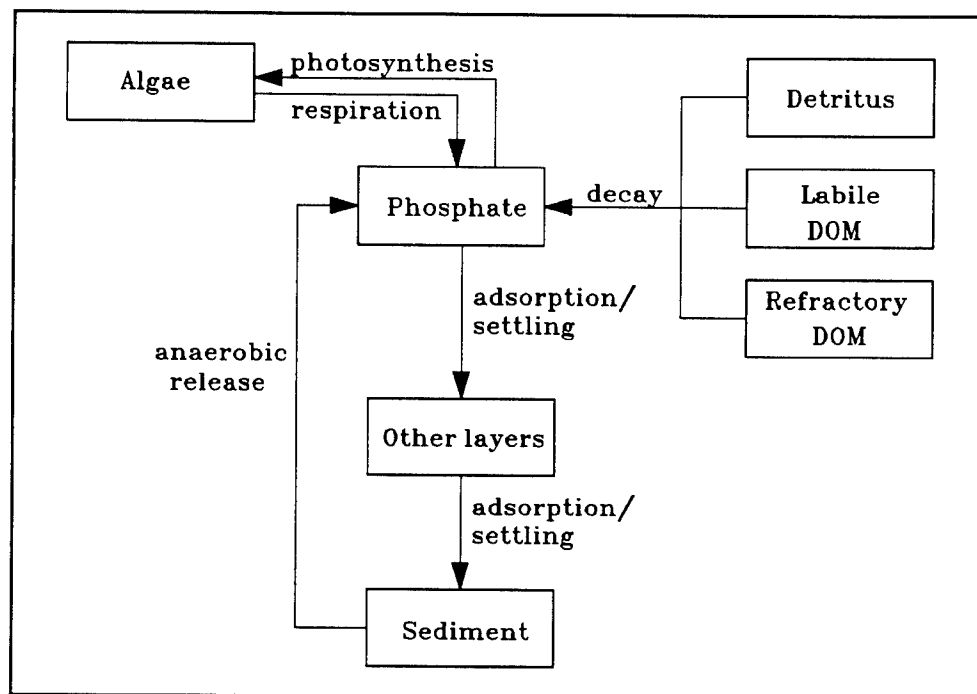
Figure B-7. Internal flux between phosphorus and other compartments.

Referring to Figure B-7, the rate equation for phosphorus is:

$$\frac{\partial \Phi_P}{\partial t} = (K_{ar} - K_{ag})\delta_P \Phi_a + K_{ldom}\delta_P \gamma_{om} \Phi_{ldom} + K_{dt}\delta_P \gamma_{om} \Phi_{dt}$$

$$+ K_{rdom}\delta_P \gamma_{om} \Phi_{rdom} + K_s \delta_P \gamma_{om} \Phi_s + S_{od}\gamma_{om}\gamma_{om} A_s \qquad (B-15)$$

$$- \frac{P_P(\omega_{ss}\Phi_{ss} + \omega_{dt}\Phi_{dt} + \omega_{FE}\Phi_{FE})}{\Delta z}\Phi_P$$

where

Δz = model cell thickness, m

A_s = sediment area, m^2

P_P = adsorption coefficient, $m^3\ g^{-1}$

δ_P = stoichiometric coefficient for phosphorus

γ_{om} = temperature rate multiplier for organic matter decay

ω_i = settling velocities, $m\ sec^{-1}$

K_{ar} = algal dark respiration rate, sec^{-1} (see equation B-11)

K_{ag} = algal growth rate, sec^{-1} (see equation B-6)

K_{ldom} = labile DOM decay rate, sec^{-1}

K_{dt} = detritus decay rate, sec^{-1}

K_s = sediment decay rate, sec^{-1}

S_{od} = anaerobic sediment release rate, $g\ m^{-3}$

K_{rdom} = refractory DOM decay rate, sec^{-1}

Φ_{rdom} = refractory DOM concentration, $g\ m^{-3}$

Φ_a = algal concentration, $g\ m^{-3}$

Φ_{ldom} = labile DOM concentration, $g\ m^{-3}$

Φ_{dt} = detritus concentration, $g\ m^{-3}$

Φ_s = organic sediment mass, g

Φ_{ss} = inorganic suspended solids concentration, $g\ m^{-3}$

Φ_P = phosphorus concentration, $g\ m^{-3}$

Φ_{FE} = total iron concentration, $g\ m^{-3}$

and the rate terms are evaluated in subroutine PHOSPHORUS.

The contribution of algae, detritus, and DOM to phosphorus is given in the rate equations and Figure B-7. However, effects due to settling and contribution from sediments require some additional explanation.

Phosphorus adsorbs onto particulates under oxic conditions and is lost when these materials settle. Loss may be rapid in the upper end of reservoirs (riverine and transition zones) due to greater concentrations of allochthonous particu-

lates. Loss occurs at a slower rate in the lacustrine zone as phosphorus adsorbs onto authochthonous particulates which may settle at a slower rate. A Langmuir isotherm describes this process. Since phosphorus concentrations are generally small, only the isotherm's linear region is utilized and is represented by the product $P_P\Phi_P$. The adsorbed solids settle at a rate equal to the solids' settling velocity. Adsorption is not allowed to occur if dissolved oxygen concentrations are less than a minimum value [O2LIM] (see page C106).

Sediment contribution of phosphorus to overlying waters can be simulated in three ways. In the first, the sediment compartment accumulates detritus and algae which then decay. This is modeled as a first-order process. However, sediment phosphorus release depends upon sediment age, chemistry, overlying phosphorus concentrations, and other factors not included in the sediment compartment. In the second, sediments can be assigned a release rate for phosphorus that is independent of sediment concentrations. Sediments are modeled as a "black box" using a zero-order rate. Phosphorus release is only allowed to occur if the overlying water dissolved oxygen concentration is less than a minimum value [O2LIM] (see page C106). The third method is a combination of the first two where organic materials accumulate and decay in the sediments along with a background decay rate independent of organic matter accumulation in the sediments.

Ammonia-Nitrogen

Ammonia-nitrogen is used by algae during photosynthesis to form proteins. In many estuarine applications, nitrogen is the limiting nutrient for algal growth.

Referring to Figure B-8, the rate equation for ammonia-nitrogen is:

$$\frac{\partial \Phi_{NH4}}{\partial t} = K_{ar}\delta_N\Phi_s - K_{ag}\delta_N\Phi_a \frac{\Phi_{NH4}}{\Phi_{NH4}+\Phi_{NO3}} + K_{ldom}\delta_N\gamma_{om}\Phi_{ldom}$$

$$+ K_{rdom}\delta_N\gamma_{om}\Phi_{rdom} + K_{dt}\delta_N\gamma_{om}\Phi_{dt} + K_s\delta_N\gamma_{om}\Phi_s$$

$$+ S_{NH4}\gamma_{om}A_s + K_{NO3}\gamma_{NO3}\Phi_{NO3} - K_{NH4}\gamma_{NH4}\Phi_{NH4}$$

(B-16)

where

A_s = sediment area, m^3
Δz = cell thickness, m
δ_N = stoichiometric coefficient for nitrogen
γ_{om} = temperature rate multipliers for organic matter decay
γ_{NH4} = temperature rate multiplier for nitrification
γ_{NO3} = temperature rate multiplier for denitrification
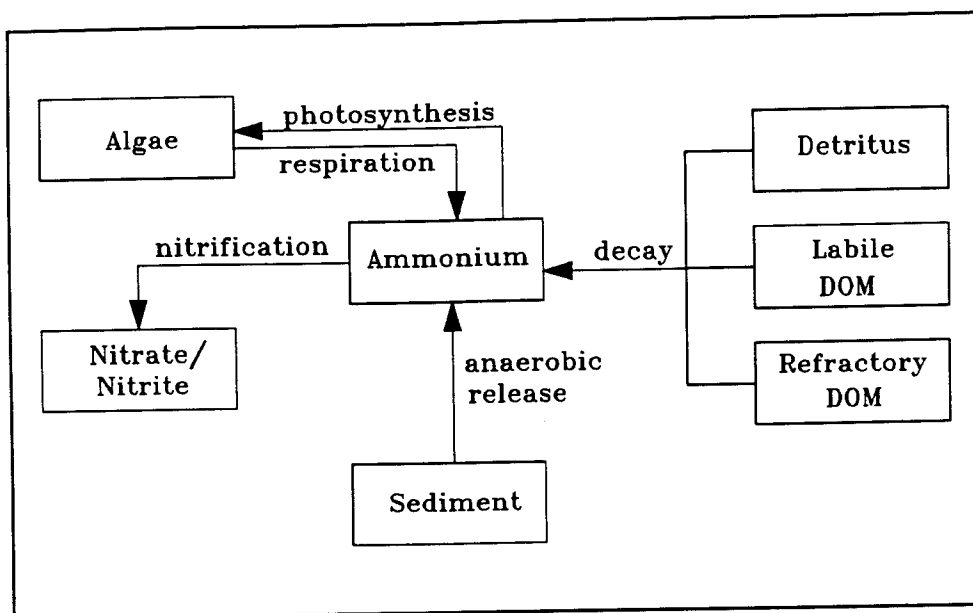
Figure B-8. Internal flux between ammonia-nitrogen and other compartments.

K_{ar} = algal dark respiration rate, sec^{-1} (see equation B-11)

K_{ag} = algal growth rate, sec^{-1} (see equation B-6)

K_{ldom} = labile DOM decay rate, sec^{-1}

K_{rdom} = refractory DOM decay rate, sec^{-1}

K_{dt} = detritus decay rate, sec^{-1}

K_s = sediment decay rate, sec^{-1}

S_{NH4} = sediment ammonia release rate, $g\ m^{-2}\ sec^{-1}$

K_{NO3} = nitrate-nitrogen decay rate, sec^{-1}

K_{NH4} = ammonia-nitrogen decay rate, sec^{-1}

Φ_{ss} = suspended solids concentration, $g\ m^{-3}$

Φ_{ldom} = labile DOM, $g\ m^{-3}$

Φ_{rdom} = refractory DOM, $g\ m^{-3}$

Φ_a = algal concentration, $g\ m^{-3}$

Φ_{dt} = detritus concentration, $g\ m^{-3}$

Φ_{NH4} = ammonia-nitrogen concentration, $g\ m^{-3}$

Φ_{NO3} = nitrate-nitrogen concentration, $g\ m^{-3}$

Φ_s = sediment mass, g

and the rate terms are evaluated in subroutine AMMONIA. As with phosphorus, zero-order sediment release only occurs when dissolved oxygen is less than a minimum value [O2LIM] (see page C106). Either a zero- or first-order process or a combination of both may be used for sediment ammonia release.

Nitrate-Nitrogen

This compartment represents nitrate plus nitrite-nitrogen. Nitrite is an intermediate product in nitrification between ammonium and nitrate. Nitrate is used as a source of nitrogen for algae and macrophytes during photosynthesis.

Nitrogen may be the limiting nutrient for algae in systems with high phosphorus loadings or in estuaries. Some species of blue-green algae are capable of fixing atmospheric nitrogen for use in photosynthesis. Nitrogen fixation is not in the model, so simulations dominated by nitrogen-fixing blue-green algae should be interpreted cautiously.
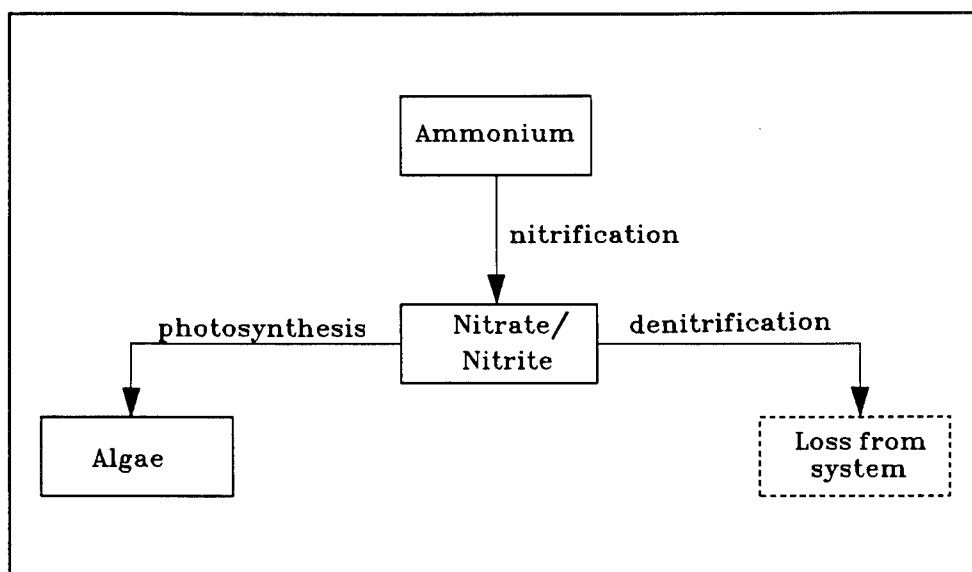
Figure B-9. Internal flux between nitrate + nitrite-nitrogen and other compartments.

Referring to Figure B-9, the rate equation for nitrate-nitrogen is:

$$\frac{\partial \Phi_{NO3}}{\partial t} = K_{NH4}\gamma_{NH4}\Phi_{NH4} - K_{NO3}\gamma_{NO3}\Phi_{NO3}$$

$$- K_{ag}\delta_N\Phi_a \left[1 - \frac{\Phi_{NH4}}{\Phi_{NH4} + \Phi_{NO3}} \right] \tag{B-17}$$

where

γ_{NH4} = temperature rate multiplier for nitrification
γ_{NO3} = temperature rate multiplier for denitrification
δ_N = stoichiometric coefficient for nitrogen
K_{NH4} = nitrification rate, sec^{-1}
K_{NO3} = denitrification rate, sec^{-1}
K_{ag} = algal growth rate, sec^{-1} (see equation B-6)
Φ_a = algal concentration, $g\ m^{-3}$
Φ_{NH4} = ammonia-nitrogen concentration, $g\ m^{-3}$
Φ_{NO3} = nitrate-nitrogen concentration, $g\ m^{-3}$

and the rate terms are evaluated in subroutine NITRATE. Nitrification is only allowed to occur if oxygen is present, and denitrification is allowed only if dissolved oxygen is less than a specified minimum value [O2LIM] (see page C106).

Dissolved Oxygen

Oxygen is one of the most important elements in aquatic ecosystems. It is essential for higher forms of life, controls many chemical reactions through oxidation, and is a surrogate variable indicating the general health of aquatic systems.

CE-QUAL-W2 includes both aerobic and anaerobic processes. The ability to model anaerobic periods is important since it provides information on potential problems with water quality. Simulations can be used to identify possibilities for both metalimnetic and hypolimnetic oxygen depletion and its impact on various water control management alternatives. If a single variable were to be measured in aquatic systems that would provide maximum information about the system state, it would be dissolved oxygen.

Referring to Figure B-10, the rate equation for dissolved oxygen is:

$$\frac{\partial \Phi_{DO}}{\partial t} = K_{ag}\delta_{om}\Phi_a - K_{ar}\delta_{om}\Phi_a - K_{NH4}\delta_{NH4}\gamma_{NH4}\Phi_{NH4}$$

$$- K_{dt}\delta_{om}\gamma_{om}\Phi_{dt} - K_s\delta_{om}\gamma_{om}\Phi_s - S_{od}\gamma_{om}A_s \qquad (B-18)$$

$$- K_{ldom}\gamma_{om}\delta_{om}\Phi_{ldom} - K_r\delta_{om}\gamma_{om}\Phi_{rdom} + A_{kt}E_o(\Phi'_{DO} - \Phi_{DO})$$

where

A_s = sediment surface area, m^2

A_{kt} = water surface surface area, m^2

δ_{om} = oxygen stoichiometric coefficient for organic matter

δ_{NH4} = oxygen stoichiometric coefficient for nitrification

γ_{NH4} = temperature rate multiplier for nitrification

γ_{om} = temperature rate multiplier for organic matter decay

K_{ag} = algal growth rate, sec^{-1} (see equation B-6)

K_{rs} = algal dark respiration rate, sec^{-1} (see equation B-11)

K_a = ammonia decay (nitrification) rate, sec^{-1}

K_{dt} = detritus decay rate, sec^{-1}

K_{ldom} = labile DOM decay rate, sec^{-1}

K_{rdom} = refractory DOM decay rate, sec^{-1}

K_s = sediment decay rate, sec^{-1}

S_{od} = sediment oxygen demand, $g\ m^{-2}\ sec^{-1}$

E_o = interfacial exchange rate for oxygen, $m\ sec^{-1}$

C_a = algal concentration, $g\ m^{-3}$

Φ_{ldom} = labile DOM concentration, $g\ m^{-3}$

Φ_{rdom} = refractory DOM concentration, $g\ m^{-3}$

Φ_{dt} = detritus concentration, $g\ m^{-3}$

Φ_{NH4} = ammonia-nitrogen concentration, $g\ m^{-3}$

Φ_{DO} = dissolved oxygen concentration, $g\ m^{-3}$

Φ_s = sediment mass, g

Φ'_{DO} = saturation DO concentration, $g\ m^{-3}$ (see equation B-22)

and the rate terms are evaluated in subroutine DISSOLVED_OXYGEN. Decay is not allowed to occur when dissolved oxygen concentrations are zero. This is accomplished by setting temperature rate multipliers equal to zero.
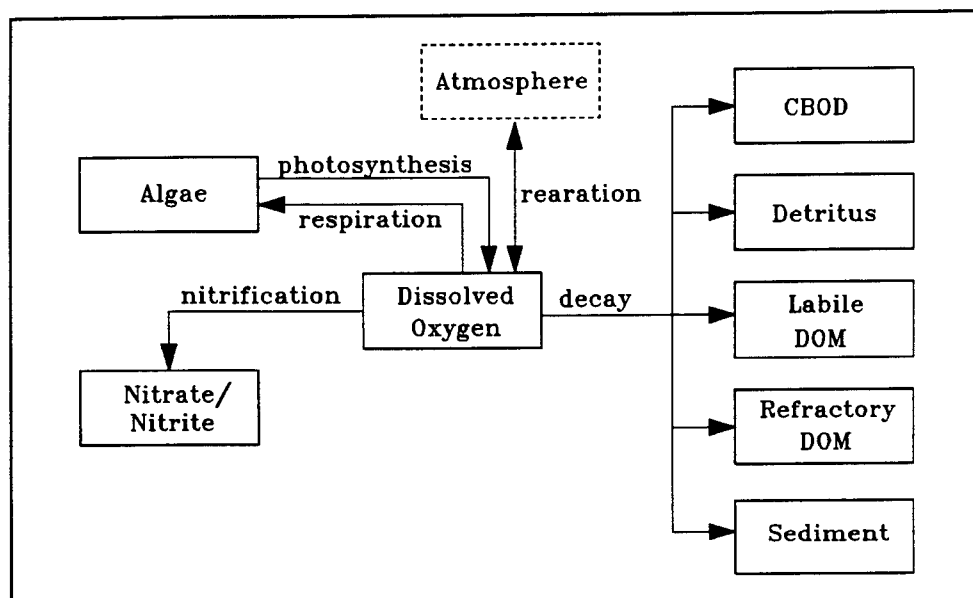
Figure B-10.   Internal flux between dissolved oxygen and other compartments.

The interfacial exchange rate is computed according to Kanwischer (1963):

$$E_o = \frac{D_o}{\left[200 - 60\sqrt{W_a}\right] \times 10^{-6}} \qquad \text{(B-19)}$$

where

D_o = molecular diffusivity of dissolved oxygen
W_a = wind speed, $m\ sec^{-1}$

W_a is limited to 11 m sec^{-1} to avoid instabilities. An alternative expression from Mackay (1980, as reported in Chapra and Reckhow 1983) is:

$$E_o = 6.4185 \times 10^{-6} \frac{W_a^{1.5}}{\sqrt{M_{O2}}} \qquad \text{(B-20)}$$

where

M_{O2} = molecular weight of oxygen

The FORTRAN code must be changed in subroutine DISSOLVED_OXYGEN to use this formulation.

Saturation dissolved oxygen is calculated from Mortimer (1981)

$$\Phi'_{DO} = e^{\left(7.7117 - 1.31403\,\{\ln\,(T_s + 45.93)\}\right)} \qquad\qquad \text{(B-21)}$$

where

$\quad$ T_s = surface water temperature, °C
Φ'_{DO} = saturation dissolved oxygen concentration, $g\ m^{-3}$

Saturation concentration is corrected for altitude by:

$$\Phi'_{DO} = \Phi_{DO} \left[1 - \frac{H}{44.3} \right]^{5.25} \qquad\qquad \text{(B-22)}$$

where

$\quad$ H = reservoir altitude, km

Sediments

Organic sediment contributions to nutrients and dissolved oxygen demand is simulated in two ways in the model. The first method uses a constant, or zero-order, release and demand. This method has been frequently used to model sediment demands and release rates. It does not depend on sediment concentrations or require a separate sediment compartment. However, the formulation is not predictive. As a consequence, results should be interpreted cautiously when evaluating effects of different nutrient loadings on dissolved oxygen in a waterbody.

The second method uses a sediment compartment to accumulate organic sediments and allow their decay. Nutrient releases and oxygen demand are thus dependent upon sediment accumulation - a first-order process. However, there is no accumulation of phosphorus or other diagenesis products when overlying water is oxic. Version 3.0 will include a fully predictive sediment model. Either of these methods, or a combination, may be used to simulate effects of organic sediments upon water quality. Again, caution must be exercised to avoid errors if both pathways are used.

The zero-order process uses a specified sediment oxygen demand and release rates for phosphorus, ammonia-nitrogen, and iron which are temperature depen
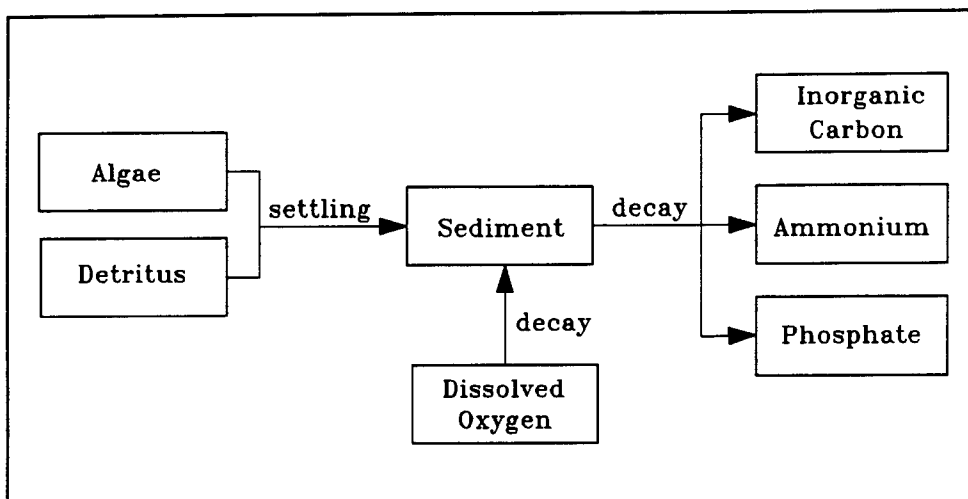
Figure B-11.   Internal flux between organic sediments and other compartments.

dent. Decay and nutrient releases do not occur when dissolved oxygen concentrations are above a minimum value [O2LIM] (see page C106). The sediment contribution to inorganic carbon is computed as a fraction of the sediment oxygen demand.

The first-order process requires specifying inclusion of this compartment in the simulation, a decay rate, and initial conditions. The sediment compartment is not transported. Instead, a compartmental equation is written for the sediment compartment which is solved within the subroutine SEDIMENT.

Referring to Figure B-11, the compartment equation for organic sediment is:

$$\frac{d\Phi_s}{dt} = \frac{\omega_{dt}}{\Delta z}\Phi_{dt} + \frac{\omega_a}{\Delta z}\Phi_a - \gamma_{om}K_s\Phi_s \qquad (B-23)$$

where

Δz = model cell thickness, m
ω_{dt} = detritus settling velocity, $m\ sec^{-1}$
ω_a = algal settling velocity, $m\ sec^{-1}$
γ_{om} = rate multiplier for organic matter
K_s = sediment decay rate, sec^{-1}
Φ_a = algal concentration, $g\ m^{-3}$
Φ_{dt} = detritus concentration, $g\ m^{-3}$
Φ_s = sediment mass, g

Total Inorganic Carbon

Carbon, hydrogen, and oxygen are the most abundant elements in living matter and form the essential backbone of organic material. Inorganic carbon directly influences pH.

Referring to Figure Figure B-12, the rate equation for total inorganic carbon is:

$$\frac{\partial \Phi_{tic}}{\partial t} = (K_{ar} - K_{ag})\delta_C\Phi_a + K_{dt}\delta_C\gamma_{om}\Phi_{dt} + K_s\gamma_{om}\delta_C\Phi_s$$
$$+ K_{ldom}\gamma_{om}\delta_C\Phi_{ldom} + K_{rdom}\gamma_{om}\delta_C\Phi_{rdom} \qquad \text{(B-24)}$$
$$+ S_{od}\gamma_{om}\delta_s A_s + A_{kt} E_c (\Phi'_{CO2} - \Phi_{CO2})$$

where

A_s = sediment surface area, m^2
A_{kt} = surface area of top cell, m^2
γ_{ii} = temperature rate multipliers
δ_C = stoichiometric coefficients for carbon
K_{ar} = algal dark respiration rate, sec^{-1} (see equation B-11)
K_{ag} = algal growth rate, sec^{-1} (see equation B-6)
K_{dt} = detritus decay rate, sec^{-1}
K_s = sediment decay rate, sec^{-1}
K_{ldom} = labile DOM decay rate, sec^{-1}
K_{rdom} = refractory DOM decay rate, sec^{-1}
S_{od} = sediment oxygen demand, $g\ m^{-2}\ sec^{-1}$
E_c = inorganic carbon interfacial exchange rate, $m\ sec^{-1}$
Φ_{ldom} = labile DOM concentration, $g\ m^{-3}$
Φ_{rdom} = refractory DOM concentration, $g\ m^{-3}$
Φ_a = algal concentration, $g\ m^{-3}$
Φ_{dt} = detritus concentration, $g\ m^{-3}$
Φ_s = sediment mass, g
Φ_{tic} = inorganic carbon concentration, $g\ m^{-3}$
Φ_{CO2} = carbon dioxide concentration, $g\ m^{-3}$
Φ'_{CO2} = carbon dioxide saturation concentration, $g\ m^{-3}$ (see equation B-27)

and the rate terms are evaluated in subroutine INORGANIC_CARBON.
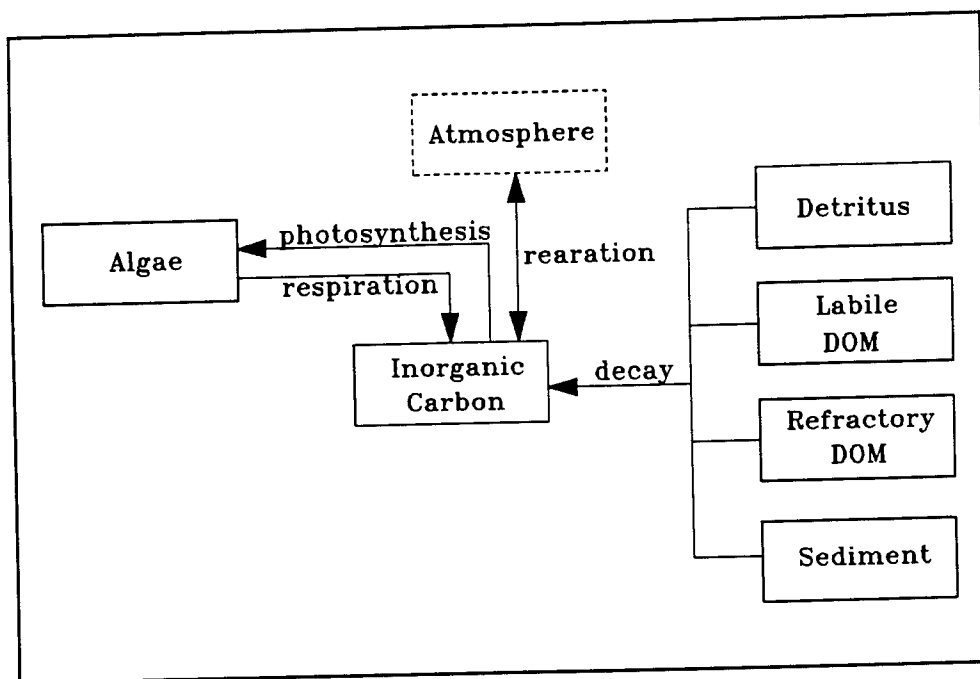
Figure B-12. Internal flux between inorganic carbon and other compartments.

Interfacial exchange is computed from Kanwischer (1963):

$$E_c = \frac{D_c}{\left[200 - 60\sqrt{W_a}\right] \times 10^{-6}} \qquad \text{(B-25)}$$

where

D_c = molecular diffusivity of carbon dioxide

W_a = wind speed, $m\ sec^{-1}$

An alternative expression from Mackay (1980, in Chapra and Reckhow 1983) can also be used:

$$E_c = 6.4185 \times 10^{-6}\ \frac{W_a^{1.5}}{\sqrt{M_{CO2}}} \qquad \text{(B-26)}$$

where

M_{CO2} = molecular weight of carbon dioxide

Appropriate coding must be substituted to use this or another formula.

Carbon dioxide concentration for the interfacial exchange rate is determined from total inorganic carbon and alkalinity in subroutine PH_CO2. The saturation concentration of carbon dioxide is determined from:

$$\Phi'_{CO2} = 0.286 \, e^{(-0.0314\,T)} P_a \tag{B-27}$$

where

P_a = altitude correction factor
T_s = surface cell water temperature, $°C$

Altitude correction is from Mortimer, 1981:

$$P_a = \left[1 - \frac{H}{44.3} \right]^{5.25} \tag{B-28}$$

where

H = reservoir elevation from sea level, *km*

Alkalinity

Alkalinity provides an indication of the buffering capacity of aquatic systems and their resistance to pH changes from acidic or alkaline loadings. Alkalinity is treated as conservative in the model and its internal rate term is set to zero. Alkalinity, along with total inorganic carbon, is used to determine pH and concentrations of carbonate species in subroutine PH_CO2.

In reality, alkalinity variations are common in most aquatic systems. Whitings, or large precipitations of carbonates, may occur. Sediment release of carbonates may increase alkalinity in the anoxic zones of many reservoirs. If these effects are important, a non-conservative model of alkalinity should be added. Version 3.0 will include a non-conservative algorithm for alkalinity.

pH and Carbonate Species

The pH and carbonate species are computed using water temperature, TDS or salinity, alkalinity, and total inorganic carbon concentrations using basic carbonate relationships. Computed carbonate species are carbon dioxide, bicarbonates, and carbonates. The pH and carbonate species are computed in subroutine

PH_CO2. These materials are not subject to transport and are computed at each water quality update interval.

Calculations performed by subroutine PH_CO2 are based on the carbonate--bicarbonate equilibrium reaction (Stumm and Morgan 1981):

$$CO_2 + H_2O \; \leftrightharpoons \; H_2CO_3 \; \leftrightharpoons \; H^+ + HCO_3^- \tag{B-29}$$

$$HCO_3^- \; \leftrightharpoons \; CO_3^- + H_+ \tag{B-30}$$

$$H_2O \; \leftrightharpoons \; H^+ + OH^- \tag{B-31}$$
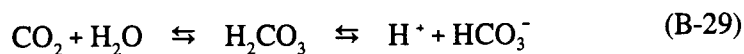
These equilibria express the source of bicarbonate and carbonate ions, alkaline constituents, and dissolution of atmospheric CO_2 in water. Contribution of calcium and magnesium carbonate to alkalinity is not included. The equilibrium state in terms of the equilibrium constants K_i is:

$$K_1 = \frac{[H^+][HCO_3^-]}{[H_2CO_3]} \tag{B-32}$$

$$K_2 = \frac{[H^+][CO_3^-]}{[HCO_3^-]} \tag{B-33}$$

$$K_w = \frac{[H^+][OH^-]}{[H_2O]} \tag{B-34}$$

where

$[X]$ = molar concentration of X
$[H20]$ = unity (by definition)

Alkalinity is defined as:

$$[ALK] = [HCO_3^-] + 2[CO_3^-] + [OH^-] - [H^+] \qquad \text{(B-35)}$$

The following condition prevails for the dissolution of carbonic acid:

$$[H_2CO_3] + [HCO_3^-] + [CO_3^-] = CONSTANT = C_T \qquad \text{(B-36)}$$

By combining equations B-32, B-33, and B-36, the quantities $[HCO_3^-]$ and $[CO_3^=]$ can be expressed in terms of $[H^+]$ and the constant C_T. In addition, equation B-34 allows for $[OH^-]$ to be expressed in terms of $[H^+]$. When these expressions are included in equation B-35, the result is:

$$[ALK] = \frac{C_T[H^+]K_1}{[H^+]K_1 + K_1K_2 + [H^+]^2} \frac{[H^+]+2K_2}{[H^+]} + \frac{K_w}{[H^+]} - [H^+] \qquad \text{(B-37)}$$

The model interprets the constant C_T as moles per liter of total inorganic carbon and assumes $[ALK]$ is known. Equation B-37 is iteratively solved in subroutine PH_CO2 until the value of $[H^+]$ converges. The negative logarithm of $[H^+]$ is, by definition, pH.

Once equation B-37 has been solved for $[H^+]$, then $[H_2CO_3]$ is given by:

$$[H_2CO_3] = \frac{C_T}{1 + \dfrac{K_1}{[H^+]} + \dfrac{K_1K_2}{[H^+]^2}} \qquad \text{(B-38)}$$

and is the same as $[CO_2]$. Bicarbonate concentration is computed from:

$$[HCO_3^-] = \frac{C_T}{1 + \dfrac{[H^+]}{K_1} + \dfrac{K_2}{[H^+]}} \qquad \text{(B-39)}$$

and carbonate from:

$$[CO_3^-] = \frac{C_T}{1 + \frac{[H^+]^2}{K_1 K_2} + \frac{[H^+]}{K_2}}$$ (B-40)

which are then converted to grams per cubic meter.

Equilibrium constants in the preceding equations are obtained by first expressing a thermodynamic temperature dependence for a related constant, K_i^*:

$$\log K_i^* = a + \frac{b}{T} + cT + d \log T$$ (B-41)

The constants a, b, c, and d are:

	a	b	c	d
K_w^*	35.3944	-5242.39	-0.00835	11.8261
K_1^*	14.8435	-3404.71	-0.03278	0
K_2^*	6.4980	-2902.39	-0.02379	0

The relation between K_i and K_i^* is obtained from the definition of the activity of a chemical species:

$$\{X\} = \gamma [X]$$ (B-42)

where

$\{X\}$ = activity of species X, *moles liter^{-1}*
γ = dimensionless activity coefficient
$[X]$ = concentration, *moles litre^{-1}*

For the reaction:

$$A + B \rightleftharpoons C + D \qquad \text{(B-43)}$$

the equilibrium constant K^* is:

$$K^* = \frac{\{C\}}{\{A\}} \frac{\{D\}}{\{B\}} \qquad \text{(B-44)}$$

thus:

$$K^* = \frac{\gamma_C [C] \gamma_D [D]}{\gamma_A [A] \gamma_B [B]} = \frac{\gamma_C \gamma_D}{\gamma_A \gamma_B} K \qquad \text{(B-45)}$$

$$K = \frac{\gamma_A \gamma_B}{\gamma_C \gamma_D} K^* \qquad \text{(B-46)}$$

Activity coefficients are obtained from an extension of Debye-Huckel theory as:

$$\text{Log}\,\gamma = \frac{-AZ^2\sqrt{I}}{1 + 0.33a\sqrt{I}} + k_1 + k_2 I + k_3 I^2 \qquad \text{(B-47)}$$

where

I = ionic strength
Z = ionic charge
A = approximately 0.5 for water at 25° C
a = ionic size parameter
k_i = empirical coefficients

Ionic strength is approximated as (Sawyer and McCarty 1967):

$$I = 2.5 \times 10^{-5} \times \Phi_{TDS} \qquad \text{(B-48)}$$

or for salinity:

$$I = 0.00147 + 0.019885 \Phi_{sal} + 0.000038 \Phi_{sal}^2 \qquad \text{(B-49)}$$

where

Φ_{TDS} = total dissolved solids, $g\ m^{-3}$
Φ_{sal} = salinity, kg m^{-3}

Values of the other parameters are:

	Z	a	k_1	k_2	k_3
HCO_3^-	1	4	0.0047	0.042	-0.0093
$CO_3^=$	2	4.5	0.0121	0.0972	-0.0207

Activity coefficients for $[H^+]$, $[OH^-]$, $[H_2CO_3]$, and $[H_2O]$ are treated as special cases:

$$[H^+]\ \gamma = [H_2O]\ \gamma = 1$$
$$[H_2CO_3]\ \gamma = [OH^-]\ \gamma = 0.0755I$$

Total Iron

Total iron is included in the model primarily because of its effect on nutrient concentrations through adsorption and settling. Iron is commonly released from anoxic sediments and may influence nutrient dynamics in many reservoirs. Iron may also contribute to dissolved oxygen depletions, but the model does not presently include these effects. Iron sediment release is modeled as a zero-order process.

Referring to Figure B-13, the rate equation for total iron is:

$$\frac{\partial \Phi_{FE}}{\partial t} = S_{FE}\gamma_{om}A_s - \frac{\omega_{FE}}{\Delta z}\Phi_{FE} \qquad (B-50)$$

where

A_s = sediment area, m^2
Δz = cell thickness, m
γ_{om} = temperature rate multiplier
ω_{FE} = settling velocity, $m\ sec^{-1}$
S_{FE} = sediment release rate, $g\ m^{-2}\ sec^{-1}$
Φ_{FE} = total iron concentration, $g\ m^{-3}$

and the rate terms are evaluated in subroutine TOTAL_IRON.
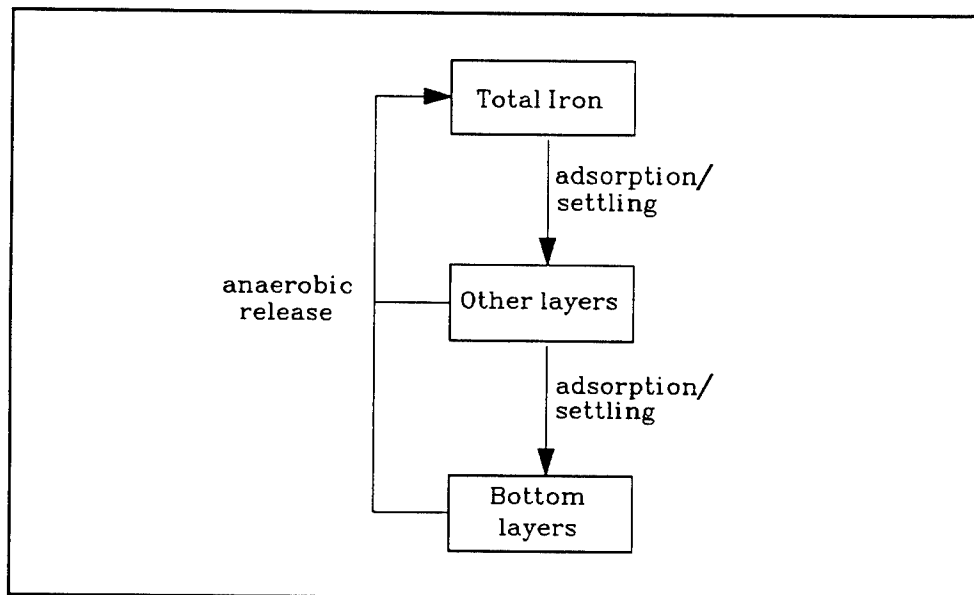
Figure B-13. Internal flux between total iron and other compartments.

Temperature Rate Multipliers

Most biological and chemical rates are temperature dependent. Subroutine RATE_MULTIPLIERS calculates the temperature dependence for all rates. It is called after the temperature solution so the temperature of the current computational interval is used.

A representative rate multiplier function is shown in Figure B-14 with its K and T parameters. The curve shape represents how biological process rates exhibit an optimum range and diminish (asymmetrically) at higher and lower temperatures (Thornton and Lessem 1978).

$$\lambda_{ii} = 0 \qquad\qquad\qquad\qquad\qquad\qquad \text{when} \quad T \leq T_1$$

$$\lambda_{ii} = \frac{K_1 e^{\gamma_1 (T-T_1)}}{1 + K_1 e^{\gamma_1 (T-T_1)} - 1} \quad \frac{K_4 e^{\gamma_2 (T_4 - T)}}{1 + K_4 e^{\gamma_2 (T_4 - T)} - 1} \quad \text{when} \quad T_1 < T < T_4 \quad \text{(B-51)}$$

$$\lambda_{ii} = 0 \qquad\qquad\qquad\qquad\qquad\qquad \text{when} \quad T \geq T_4$$

where

$$\gamma_1 = \frac{1}{T_2 - T_1} \; \ln \frac{K_2 (1 - K_1)}{K_1 (1 - K_2)}$$

$$\gamma_2 = \frac{1}{T_4 - T_3} \; \ln \frac{K_3 (1 - K_4)}{K_4 (1 - K_3)}$$

The user supplies temperatures T_1 to T_4 and multiplier factors K_1 to K_4. Temperatures T_1 and T_4 represent mortality limits, and T_2 and T_3 are used to define the optimum range. Maximum reaction rates supplied by the user are multiplied by λ_{ii} to determine rates corresponding to the water temperature of a model cell.
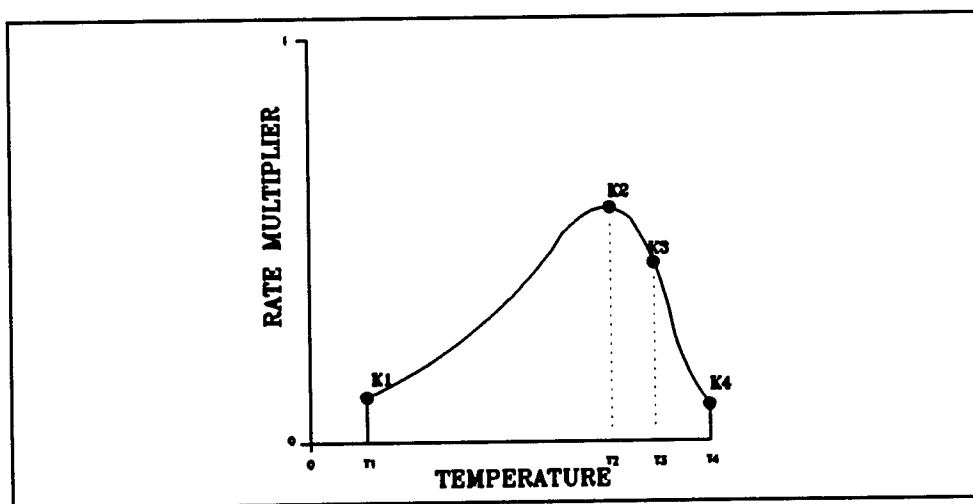
Figure B-14. Temperature rate multiplier function.

Appendix C
Input Data Description

Input file format has been developed for a full-screen text editor. Each input file begins with two lines used for file identification which are ignored by the program. The rest of the input file consists of groups of three lines - the first line is blank serving as a separator, the second line contains the card identification and the FORTRAN variable names associated with the input card, and the third line contains the input values. The identifier card is only checked by the pre-processor code. FORTRAN names are right justified according to the field widths associated with the input variable. There are 10 input fields associated with each card although the first field is not used in several of the input files. Each field has a length of eight characters.

Control File

The control file [CONFN] contains the variables used to run the model. There are no optional cards in the control file - each card is *required* although there may be either zero or 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. An example of a portion of the control file for the DeGray Lake case (or in some instances, another application to illustrate features not used in the DeGray Lake application) is given with each card description.

Title (TITLE C)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TITLE	Character	Text for identification of simulation

There are six title cards that can be used to identify various types of output. Each line may contain up to 72 characters of text. Title cards appear in every output file except for the restart file. Uses for the title cards include identifying the simulation, the simulation time frame, the date the simulation was run, and other information specific to the simulation. A few words of wisdom - the user should be conscientious in updating the title cards for each simulation.

Example

```
TITLE C .............................TITLE....................................
        J. Strom Thurmond Lake - scenario run 1
        Proposed summer power generation schedule
        No pumpback or channel improvement
        High Pool Elevation
        Stations @ 0.25, 1.25, 2.25, 3.25, 5,75, and 6.75 km from RBR dam
        Test run
```

Time Control (TIME CON)

Field	Name	Value	Description
1			(Ignored by code)
2	TMSTRT	Real	Starting time, *Julian day*
3	TMEND	Real	Ending time, *Julian day*
4	YEAR	Real	Starting year

The simulation starting and ending times are specified with this card. When making a simulation extending into another year, the ending time is calculated as 364 (or 365 for a leap year) + Julian date of ending time. January 1 starts at Julian day 0.0 in the model. This is a different concept than what is usually employed for Julian dates. For example, 12 noon on January 1 would correspond to Julian day 0.5 in the model. Twelve midnight on January 1 would correspond to Julian day 1.0. This is necessary since fractions of Julian days exist in the model.

Example

```
TIME CON  TMSTRT   TMEND    YEAR
          63.5     64.5     1980
```

Timestep Control (DLT CON)

Field	Name	Value	Description
1			(Ignored by code)
2	NDT	Integer	Number of timestep intervals
3	MINDLT	Real	Minimum timestep, *sec*

The number of timestep intervals and minimum timestep are specified on this card.

The autostepping algorithm calculates a maximum timestep based on hydrodymanic numerical stability requirements (see page D26) and then uses a fraction of this value for the actual timestep. The user can specify up to 50 intervals in which the maximum timestep and fraction of the timestep can vary. These values are specified in the next three cards. This option is useful during periods of very low flow where the timestep is very large. Under these conditions, small changes in flow will result in large timestep changes which can lead to an excessive number of timestep violations detected by the autostepping algorithm. Also, if any inputs are at hourly intervals, then the maximum timestep should never be more than an hour. For a more detailed description of autostepping, see Appendix D, pages D26-D28.

The minimum timestep is useful during periods of extremely high flows. In these instances, the timestep could become too small to economically run the model. Care should be taken when using this variable as the model may become unstable if the minimum value is set too high.

Example

```
DLT CON     NDT  MINDLT
              1    1.0
```

Related cards and files

Timestep Interval, page C5
Maximum Timestep, page C6
Timestep Fraction, page C7

Timestep Interval (DLT DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	DLTD	Real	Beginning of timestep interval, *Julian day*

The intervals for the maximum timestep are specified on this card. Up to 50 intervals can be specified without changing the dimensions of the variables associated with the timestep interval [NDP] (Chapter 3, see page 21). If there are *more* intervals than can be specified on one line, then they are continued on the next line without another DLT DAY card being specified.

Example

```
DLT DATE    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD
            50.5    93.5   146.5   200.0   284.0
```

Related cards and files

Timestep Control, page C4
Maximum Timestep, page C6
Timestep Fraction, page C7

Maximum Timestep (DLT MAX)

Field	Name	Value	Description
1			(Ignored by code)
2-10	DLTMAX	Real	Maximum timestep, *sec*

The maximum timestep for intervals provided on the timestep interval card are specified with this card. If there are **more** intervals than can be specified on one line, then they are continued on the next line without another DLTMAX card being specified.

Example

```
DLT MAX    DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX
           1800.0  3600.0  2500.0  1800.0  3600.0
```

Related cards and files

Timestep Control, page C4
Timestep Interval, page C5
Timestep Fraction, page C7

Timestep Fraction (DLT FRN)

Field	Name	Value	Description
1			(Ignored by code)
2-10	DLTF	Real	Fraction of timestep

The fraction of the timestep for intervals given on the timestep interval card are specified here. If there are *more* intervals than can be specified on one line, then they are continued on the next line without another DLT FRN card being specified.

Example

```
DLT FRN    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF
            0.9    0.85     0.9     0.9    0.85
```

Related cards and files

Timestep Control, page C4
Timestep Interval, page C5
Maximum Timestep, page C6

Branch Geometry (BRANCH G)

Field	Name	Value	Description
1			(Ignored by code)
2	US	Integer	Branch upstream segment
3	DS	Integer	Branch downstream segment
4	UHS	Integer	Upstream boundary condition
5	DHS	Integer	Downstream boundary condition

This card specifies the branch location in the grid and branch boundary conditions. *The mainstem of the waterbody is always branch 1.* Other branches can be ordered in any fashion, but it is good practice to order the remaining branches starting with the most upstream branch and continuing downstream.

The branch upstream segment number [US] is the most upstream potentially active segment. For branch 1, this would always be segment 2. The branch downstream segment number [DS] is the most downstream *active* segment. The boundary segment is *never* included for either the upstream or downstream segment.

There are three upstream and downstream boundary conditions which can be specified. Boundary conditions along with the upstream head segment [UHS] and downstream head segment [DHS] value which specify these conditions are:

Boundary type	[UHS] and/or [DHS]
External head	-1
External flow	0
Internal head	>0

For internal head boundary conditions, [UHS] and/or [DHS] correspond to the branch segment the branch attaches to. See Chapter 3, pages 10-11 for additional information on branch setup.

The user must ensure the number of branches parameter [NBP] in the PARAMETER statement in the file W2_INC.FOR is *equal* to the number of branches in the computational grid (Chapter 3, see page 21).

Example

```
BRANCH G     US      DS      UHS     DHS     PHIO
             2       31      0       0       5.14
```

Related cards and files

Waterbody Coordinates (LOCATION)

Field	Name	Value	Description
1			(Ignored by code)
2	LAT	Real	Latitude, *degrees*
3	LONG	Real	Longitude, *degrees*
4	ELBOT	Real	

This card specifies the waterbody latitude and longitude and bottom reference elevation. The bottom elevation is used to tie computed water surface elevations to an external benchmark (e.g., m above sea level) and represents the elevation at the bottom of the bottommost active cell.

.

Example

```
LOCATION     LAT    LONG   ELBOT
             34.2   93.3   66.35
```

Initial Conditions (INIT CND)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	T2I	Real		Initial temperature, $°C$
3	ICETHI	Real		Initial ice thickness, m
4	WTYPEC	Character	FRESH	Waterbody type

This card specifies the initial temperature and ice thickness, and waterbody type. Initial temperature can be specified as either a single value, a single vertical profile used to initialize every segment, or a vertical profile for each segment.

Initial condition	[IT2]
1. Isothermal	>0
2. Single vertical profile	-1.0
3. Vertical profile at each segment	-2.0

If option 2 or 3 is chosen, then the user must specify input files [VPRFN] or [LPRFN] containing the profile(s). See pages C174-C176 for more details on the file specifications.

Initial ice thickness [ICETHI] is ignored if ice computations are turned off (see page A21, C17).

The waterbody type [WTYPEC] is either FRESH or SALT. If [WTYPEC] is set to SALT, then constituent computations [CCC] (see page C69) should be turned on and salinity should be included in the computations.

Example

```
INIT CND      T2I   ICETHI   WTYPEC
             -1.0      0.0    FRESH
```

Related cards and files

Constituent Initial Concentration, page C73
Vertical Profile File, page C174
Longitudinal Profile File, page C176
Ice Cover, page A21, C17

Calculations (CALCULAT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	VBC	Character	OFF	Volume balance calculation
3	EBC	Character	OFF	Thermal energy balance calculation
3	MBC	Character	OFF	Mass balance calculation
4	PQC	Character	OFF	Density placed inflows
5	EVC	Character	OFF	Evaporation included in water budget
6	PRC	Character	OFF	Precipitation included

This card specifies whether certain optional calculations are performed by the model. Calculations are turned on or off by *right justifying* ON or OFF in the input field.

Volume balance calculations are useful during initial runs as a check to ensure the model is preserving continuity and should always be used as a check if the user modifies the code. In order to reduce roundoff errors, the volume balance algorithm accumulates spatial and temporal *changes* in volume over time and uses these for comparison. Once the user is satisfied the model is running correctly, volume balance calculations should be turned off to reduce computational time.

Thermal energy and mass balance calculations are similar in use to volume balance calculations. They should be used initially to ensure the model is running properly and turned off for further calculations. When this option is used, mass balances are performed for each constituent if constituent computations are turned on. Mass balances are not computed if only temperature is modeled.

There are two options for distributing mainstem and branch inflows. The default is inflows distributed evenly into each layer from top to bottom. If [PQC] is turned on, then inflows are matched up with the layer(s) whose density most closely corresponds to inflow density.

If precipitation is specified, then the user must supply input files for precipitation and precipitation temperature. If constituents are being modeled, then the user must supply an input file for constituent concentrations included in the simulation. The **Precipitation Active Constituent Control** card specifies which concentrations are included (see page C78).

Evaporation rates are sometimes accounted for in estimating the inflow record. If so, then [EVC] should be set to OFF. Evaporation is *always* considered in the surface heat exchange calculations.

Example

```
CALCULAT    VBC     EBC     MBC     PQC     EVC     PRC
            ON      ON      ON      OFF     OFF     OFF
```

Related cards and files

Precipitation Active Constituent Control, page C78
Branch Inflow File, page C150
Tributary Inflow File, page C155
Precipitation File, page C161

Interpolation (INTERPOL)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	INFIC	Character	OFF	Interpolate inflows, inflow temperatures, and inflow constituent concentrations
3	TRIC	Character	OFF	Interpolate tributary inflows and inflow temperatures and constituent concentrations
4	DTRIC	Character	OFF	Interpolate distributed tributary inflows and inflow temperatures and constituent concentrations
5	HDIC	Character	OFF	Interpolate head boundary elevations and boundary temperatures and constituent concentrations
6	OUTIC	Character	OFF	Interpolate outflows
7	WDIC	Character	OFF	Interpolate withdrawals
8	METIC	Character	OFF	Interpolate meteorologic data

These options control whether time-varying data are input as a step function or linearly interpolated between data points. If interpolation is used, then the user must ensure it is appropriate and the input data supply correct information. Many reservoirs have periods of no releases. If outflow interpolation is turned on, then input data must be set up so no outflow occurs during these periods. This is accomplished by including extra dates in the outflow file with zero outflows to ensure the interpolation routine yields zero outflows. For example, given the following outflow time-series in the outflow file [QOTFN]:

```
  JDAY      QOT
 100.00    50.0
 110.00     0.0
 120.00    50.0
```

If interpolation is not used, then outflow from Julian day 100 to 110 is 50 m^{-3} sec^{-1}, from Julian day 110 to 120 is 0.0 m^{-3} sec^{-1}, and 50 m^{-3} sec^{-1} thereafter. If interpolation is turned on, then outflow linearly decreases from Julian day 100 to 110 and then increases from Julian day 110 to 120. To ensure no outflow occurs between day 110 and 120 with interpolation on, the outflow file should be setup as follows:

```
   JDAY      QOT
 100.0000   50.0
 109.9999   50.0
 110.0000    0.0
 119.9999    0.0
 120.0000   50.0
```

Example

```
INTERPOL   INFIC    TRIC   DTRIC    HDIC   OUTIC    WDIC   METIC
             ON      OFF     OFF     OFF      ON     OFF      ON
```

Related cards and files

Branch Inflow File, page C150
Tributary Inflow File, page C155
Tributary Inflow Temperature File, page C156
Tributary Inflow Concentration File, page C157
Branch Distributed Tributary Inflow File, page C158
Branch Distributed Tributary Inflow Temperature File, page C159
Branch Distributed Tributary Inflow Concentration File, page C160
Branch External Upstream Head Elevation File, page C164
Branch External Upstream Head Temperature File, page C165
Branch External Upstream Head Concentration File, page C167
Branch External Downstream Head Elevation File, page C169
Branch External Downstream Head Temperature File, page C170
Branch External Downstream Head Concentration File, page C172
Branch Outflow File, page C153
Withdrawal File, page C154
Meteorologic File, page C149

Dead Sea (DEAD SEA)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	WINDC	Character	ON	Turn on/off wind
3	QINC	Character	ON	Turn on/off all sources of water
4	QOUTC	Character	ON	Turn on/off all sinks of water
5	HEATC	Character	ON	Turn on/off heat exchange

This card has been used primarily during model development debugging. It is in the release version because it can be useful in evaluating relative effects of the hydrodynamic forcing functions and also as a debugging tool if the user decides to modify the code. Occasionaly in estuarine applications, temperature is treated conservatively with the initial and boundary conditions set at a constant temperature with bottom and heat exchange turned off although it is not recommended.

Example

```
DEAD SEA   WINDC    QINC    QOUTC    HEATC
             ON       ON       ON       ON
```

Ice Cover (ICE COVER)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	ICEC	Character	OFF	Allow ice calculations
3	SLICEC	Character	SIMPLE	Specifies the method of ice cover calculations - either SIMPLE or DETAIL
4	SLHTC	Character	ET	Specifies heat exchange solution - either ET or TERM
5	ALBEDO	Real	-	Ratio of reflection to incident radiation (albedo of ice)
6	HWI	Real	-	Coefficient of water-ice heat exchange
7	BETAI	Real	-	Fraction of solar radiation absorbed in the ice surface
8	GAMMAI	Real	-	Solar radiation extinction coefficient
9	ICEMIN	Real	-	Minimum ice thickness before ice formation is allowed, m
10	ICET2	Real	-	Temperature above which ice formation is not allowed, $^\circ C$

Ice calculations are controlled with this card. The variable [ICEC] turns on/off ice calculations. Two different methods for computing ice cover are available. The first method ([SLICEC] = SIMPLE) was included in version 1.0 and is available for backwards compatability (see page A21). The second method (DETAIL) is the preferred method (see page A22). The variable [SLHTC] species the type of heat exchange calculations used in determining surface heat exchange. This variable is used to select the method of determining surface heat exchange *even if* ice calculations are turned off. If [SLHTC] is set to TERM, then term-by-term calculations are used (see page A18). If [SLHTC] is set to ET, then equilibrium temperatures and coefficients of surface heat exchange are used to calculate surface heat exchange (see page A20).

The coefficient of water-ice heat exchange [HWI] is a user specified calibration parameter which determines the rate of heat exchange between water and ice. [BETAI] is the fraction of solar radiation absorbed at the ice surface and is similar to [BETA] in the surface heat exchange computations. [GAMMAI] is the solar radiation extinction coefficient through ice and is also similar to [GAMMA] in the surface heat exchange computations.

Albedo is the ratio of reflection to incident radiation. It is normally expressed by the albedo of a surface and varies widely depending on the solar altitude and the waterbody surface properties.

For free water surfaces, Anderson (1954), in his Lake Hefner studies, derived the following empirical formula for the water surface albedo, ALB_w, as a function of average solar altitude:

$$ALB_w = 1.18A_s^{-0.77} \qquad (B\text{-}52)$$

where A_s is average solar altitude in degrees. Anderson found the coefficient 1.18 and the exponent -0.77 to vary only slightly with cloud height and coverage.

For ice surface, a functional representation of albedo has not been established. Reported values for ice surface albedo vary greatly from about 10% for clear lake ice (Bolsenga, 1969) to almost 70% for snow free Arctic sea ice (Krutskih, et al., 1970). Krutskih, et al. suggest ice albedo is more dependent on air temperature than on solar altitude. Based on their extensive Arctic sea observations, ice surface albedo for solar radiation was determined as:

$$
\begin{aligned}
ALB_i &= \epsilon & \text{for } T_a &\leq 0°C \\
ALB_i &= \xi + \omega e^{\psi T_a} & \text{for } T_a &> 0°C
\end{aligned}
\qquad (B\text{-}53)
$$

where ϵ, ξ, ω, and Ψ are empirical constants, and T_a is air temperature, °C. Equation (B-53) is an empirical fit to the observed data given by Krutskih, et al. for Arctic ice.

Example

ICE COVER	ICEC	SLICEC	SLHTC	ALBEDO	HWI	BETAI	GAMMAI	ICEMIN	ICET2
	OFF	DETAIL	ET	0.25	10.0	0.6	0.07	0.05	3.0

Related cards and files

Initial Conditions, page C11

Transport Scheme (TRANSPORT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	SLTRC	Character	QUICKEST	Transport solution scheme - either QUICKEST or UPWIND
3	THETA	Real		Time-weighting for vertical advection scheme

This card specifies the transport solution scheme used by the model. There are two options for [SLTRC] - 'UPWIND' or 'QUICKEST' with the latter being the recommended option. The old solution scheme is retained in this version of the model mainly as a means of comparing the two solution schemes. The 'QUICKEST' option employs a higher-order solution scheme to reduce numerical diffusion present in the original 'UPWIND' differencing scheme. [THETA] specifies the amount of time-weighting in the vertical advection scheme. A value of 0 specifies fully explicit vertical advection, 1 specifies fully implicit vertical advection, and 0.55 specifies a Crank-Nicholson scheme. Vertical diffusion is always fully implicit.

Example

```
TRANSPORT  SLTRC    THETA
           QUICKEST  0.00
```

Number of Sheltering Coefficients (WSC NUMB)

Field	Name	Value	Description
1			(Ignored by code)
2	NWSC	Real	Number of time intervals the wind sheltering coefficient varies

This card specifies the number of intervals during which the wind sheltering coefficient [WSC] may vary over the simulation. The model, like the proto-type, is **extremely sensitive to wind**, and this coefficient is used to adjust the effects of the wind. Its physical basis is that surrounding terrain often shelters the waterbody so that observed winds taken from meteorologic stations are not the effective winds reaching the waterbody. Since prevailing wind direction and vegetative cover vary with time, the user has the option to vary the wind sheltering coefficient with time. Intervals and values for [WSC] are specified in the next two cards. Version 3.0 will include the option to vary wind sheltering spatially.

Example

```
WSC NUMB     NWSC
               3
```

Related cards and files

Wind Sheltering Coefficient Day, page C21
Wind Sheltering Coefficient, page C22

Wind Sheltering Coefficient Day (WSC DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	WSCD	Real	Starting time for a given wind sheltering coefficient

This card specifies time intervals during which the wind sheltering coefficient [WSC] will vary. Time intervals should roughly correspond to different seasons in which prevailing winds or vegative growth have changed sufficiently to physically justify using a different sheltering coefficient. If there are *more* dates than can be specified on one line, then they are continued on the next line without specifying another WIND DAY card.

Example

```
WSC DATE   WSCD    WSCD    WSCD    WSCD    WSCD    WSCD    WSCD    WSCD    WSCD
           50.5   160.5   240.5
```

Related cards and files

Number of Wind Sheltering Coefficients, page C20
Wind Sheltering Coefficient, page C22

Wind Sheltering Coefficient (WSC COEF)

Field	Name	Value	Description
1			(Ignored by code)
2-10	WSC	Real	Wind sheltering coefficient

This card specifies the value for the wind sheltering coefficient [WSC] which ranges from 0 to 1. The higher the value, the greater the effects of wind on the waterbody. If there are *more* coefficients than can be specified on one line, they are continued on the next line without another WIND COEF card being specified.

Example

```
WSC COEF    WSC     WSC     WSC     WSC     WSC     WSC     WSC     WSC     WSC
            1.0     0.90    0.85
```

Related cards and files

Number of Wind Sheltering Coefficients, page C20
Wind Sheltering Coefficient Day, page C21

Hydraulic Coefficients (HYD COEF)

Field	Name	Value	Description
1			(Ignored by code)
2	AX	Real	Horizontal eddy viscosity, $m^2\ sec^{-1}$
3	DX	Real	Horizontal eddy diffusivity, $m^2\ sec^{-1}$
4	CHEZY	Real	Chezy coefficient, $m^{0.5}\ sec^{-1}$
5	CBHE	Real	Coefficient of bottom heat exchange, $W\ m^{-2}\ sec^{-1}$
6	TSED	Real	Sediment (ground) temperature, $^{\circ}C$

This card specifies hydraulic and bottom heat exchange coefficients which can be varied during model calibration. The horizontal eddy viscosity [AX] specifies dispersion of momentum in the X-direction. The horizontal eddy diffusivity [DX] specifies dispersion of heat and constituents in the X-direction. Both values are presently time and space invariant. The Chezy coefficient is used in calculating effects of bottom friction. The coefficient of bottom heat exchange [CBHE] and the ground temperature [TSED] are used to compute heat exchange at the ground-water interface. Ground temperature can be estimated from average yearly temperature at the site. Recommended values are given in the example.

Previous experience has shown recommended values produce remarkably accurate temperature predictions for a wide variety of systems. The horizontal eddy viscosities and diffusivities and Chezy coefficient may need additional tuning when calibrating for water quality portion since longitudinal temperature gradients in most applications are negligable. The Chezy coefficient is important in estuarine applications for calibrating tidal range and phase. Version 3.0 will allow the Chezy coefficient to vary spatially.

Example

```
HYD COEF      AX      DX   CHEZY    CBHE     TSED
             1.0     1.0    70.0   7.0E-8    12.8
```

Selective Withdrawal (SEL WITH)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	SWC	Character	OFF	Specifies if the selective withdrawal algorithm is used in calculating outflows

This card specifies whether selective withdrawal calculations are used to determine the outflow layers for each branch. If the selective withdrawal option for a given branch is turned on, then it *overrides* any options on the N OUTLET and O LAYER cards (see pages C30-C31).

Example

```
SEL WITH    SWC     SWC     SWC     SWC     SWC     SWC     SWC     SWC     SWC
            ON      OFF     OFF
```

Related cards and files

Number of Structures, page C25
Structure Location, page C26
Sink Type, page C27
Elevation of Withdrawal Structure, page C28
Width of Withdrawal Structure, page C29

Number of Structures (N STRUC)

Field	Name	Value	Description
1			(Ignored by code)
2-10	NSTR	Integer	Number of structures for each branch

This card specifies the number of outlet structures located at the downstream segment of each branch. For example, many reservoirs have multilevel withdrawal ports. Each port would be a separate outlet structure and the total number for the branch would be entered here.

The user must ensure the number of structures parameter [NSP] in the PARAMETER statement in the file W2_INC.FOR is *equal* to the total number of structures specified on this card (Chapter 3, see page 21).

Example

```
N STRUC     NSTR     NSTR     NSTR     NSTR     NSTR     NSTR     NSTR     NSTR     NSTR
             5        0        0
```

Related cards and files

Selective Withdrawal, page C24
Structure Location, page C26
Sink Type, page C27
Elevation of Withdrawal Structure, page C28
Width of Withdrawal Structure, page C29

Bottom Layer Limit (K BOTTOM)

Field	Name	Value	Description
1			(Ignored by code)
2-10	KBSW	Integer	Bottommost layer for outflows of each structure in the selective withdrawal algorithm

The selective withdrawal algorithm calculates vertical withdrawal zone limits based on outlet geometry, outflows, and in-pool densities. The algorithm then assigns flows for each layer within the withdrawal zone. This card specifies the bottom layer for which outflows are calculated in the selective withdrawal algorithm. This option is most commonly used when a submerged weir, trash accumulation, or some other structure is located upstream from the dam which limits the bottom of the withdrawal zone.

Example

```
K BOTTOM    KBSW    KBSW    KBSW    KBSW    KBSW    KBSW    KBSW    KBSW    KBSW
Br 1         35      35      30
Br 2         20      20
```

Related cards and files

Selective Withdrawal, page C24
Number of Structures, page C25
Sink Type, page C27
Elevation of Withdrawal Structure, page C28
Width of Withdrawal Structure, page C29

Sink Type (SINK TYPE)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	SINKC	Character	LINE	Sink type used in the selective withdrawal algorithm

This card specifies the sink type for each withdrawal. The options are 'LINE' or 'POINT' each of which have different selective withdrawal characteristics (see page A27).

Line sinks are usually structures wide in relation to dam width (> 1/10). Point sinks are usually structures narrow in relation to dam width (< 1/10).

Example

```
SINK TYPE  SINKC   SINKC   SINKC   SINKC   SINKC   SINKC   SINKC   SINKC   SINKC
Br 1       POINT   POINT   LINE
Br 2       LINE    LINE
```

Related cards and files

Selective Withdrawal, page C24
Number of Structures, page C25
Structure Location, page C26
Elevation of Withdrawal Structure, page C28
Width of Withdrawal Structure, page C29

Elevation of Withdrawal Structure (E STRUC)

Field	Name	Value	Description
1			(Ignored by code)
2-10	ESTR	Real	Centerline elevation of structure, *m above msl*

This card specifies the centerline elevation for each withdrawal structure by branch.

Example

```
E STRUC    ESTR    ESTR    ESTR    ESTR    ESTR    ESTR    ESTR    ESTR    ESTR
Br 1       114.0   116.0   116.0
Br 2       111.0   114.0
```

Related cards and files

Selective Withdrawal, page C24
Number of Structures, page C25
Structure Location, page C26
Sink Type, page C27
Width of Withdrawal Structure, page C29

Width of Withdrawal Structure (W STRUC)

Field	Name	Value	Description
1			(Ignored by code)
2-10	WSTR	Real	Width of structure (line sink), *m*

This card specifies the width of the structures by branch if a link sink is specified as the sink type [SINK] (see page C27). The values are ignored if a point sink is specified.

Example

```
W STRUC    WSTR     WSTR     WSTR     WSTR     WSTR     WSTR     WSTR     WSTR     WSTR
Br 1        0.0      0.0     50.0
Br 2      100.0    500.0
```

Related cards and files

Selective Withdrawal, page C24
Number of Structures, page C25
Structure Location, page C26
Sink Type, page C27
Elevation of Withdrawal Structure, page C28

Number of Outlets (N OUTLET)

Field	Name	Value	Description
1			(Ignored by code)
2	NOUT	Integer	Total number of outlets in each branch

This card specifies the total number of outlets in the waterbody. For each outlet, a flow must be specified in the outflow file [QOTFN]. At least one outflow is required, although the flow may be set to zero. An outlet structure spanning multiple layers may be specified by breaking the single outlet into several and apportioning outflow among them. If selective withdrawal for a branch is turned on, then information on this card is ignored.

Outlets are *always* located at the most downstream segment [DS] for each branch. They are permitted only for a downstream flow boundary condition. The withdrawal option should be used for outlets not located at the downstream segment.

The user must ensure the number of structures parameter [NSP] in the PARAMETER statement in the file W2_INC.FOR is *equal* to the total number of outlets specified on this card (Chapter 3, see page 21).

Example

```
N OUTLET    NOUT    NOUT    NOUT    NOUT    NOUT    NOUT    NOUT    NOUT    NOUT
              8       3
```

Related cards and files

Outlet Layer Location, page C31
Outflow file, page C153

Outlet Layer Location (O LAYER)

Field	Name	Value	Description
1			(Ignored by code)
2-10	KOUT	Integer	Layer number for each outlet

This card specifies the layer location for each outlet. If selective withdrawal is on for a branch, then layer location information for that branch will be ignored. If the surface layer [KT] is below the level of an outlet at any time during the simulation, then outflow for that outlet is ignored. If there are *more* layer nubers than can be specified on one line, then they are continued on the next line without another O LAYER card being specified.

Example

O LAYER	KOUT	KOUT	KOUT	KOUT	KOUT	KOUT	KOUT	KOUT	KOUT
Br 1	4	5	6	7	8	9	10	11	
Br 2	5	6	7						

Related cards and files

Number of Outlets, page C30
Outflow File, page C153

Number of Withdrawals (N WDRWAL)

Field	Name	Value	Description
1			(Ignored by code)
2	NWD	Integer	Number of withdrawals

This card specifies the number of withdrawals for the waterbody. Withdrawals are associated with a layer and segment. Like outlets, withdrawal structures can span more than one layer by breaking the single withdrawal into several and apportioning outflow among them. If withdrawals are not used in the simulation, then *NWD must be set equal to zero*.

All withdrawals are considered lateral and thus are not considered in the momentum equation. The present model version cannot calculate a selective withdrawal zone for withdrawals. Version 3.0 will include this capability.

An example of a withdrawal is a water supply inlet structure. Withdrawals have also been used to simulate pumpback operations (see the JST example application supplied on the distribution disk).

The user must ensure the number of withdrawals parameter [NWP] in all the PARAMETER statement in the file W2_INC.FOR is *equal* to the total number of withdrawals specified on this card (Chapter 3, see page 21).

Example

```
N WDRWAL      NWD
               1
```

Related cards and files

Withdrawal Segment, page C33
Withdrawal Layer, page C34
Withdrawal File, page C154

Withdrawal Segment (W SEGMNT)

Field	Name	Value	Description
1			(Ignored by code)
2-10	IWD	Integer	Segment number for withdrawal

This card specifies the withdrawal segment location. If there are **more** withdrawal segments than can be specified on one line, then they are continued on the next line without another W SEGMENT card being specified.

Example

```
W SEGMNT    IWD    IWD    IWD    IWD    IWD    IWD    IWD    IWD    IWD
            20
```

Related cards and files

Number of Withdrawals, page C32
Withdrawal Layer, page C34
Withdrawal File, page C154

Withdrawal Layer (W LAYER)

Field	Name	Value	Description
1			(Ignored by code)
2-10	KWD	Integer	Layer number for withdrawal

This card specifies the withdrawal layer location. If there are **more** withdrawal layers than can be specified on one line, then they are continued on the next line without another W LAYER card being specified.

Example

```
W LAYER     KWD     KWD     KWD     KWD     KWD     KWD     KWD     KWD     KWD
              8
```

Related cards and files

Number of Withdrawals, page C32
Withdrawal Segment, page C33
Withdrawal File, page C154

Number of Tributaries (N TRIBS)

Field	Name	Value	Description
1			(Ignored by code)
2	NTR	Integer	Number of tributaries

This card specifies the number of tributaries. Tributaries are used primarily to complete the water budget without having to include tributaries in the computational grid. They can also be used to represent point source loadings.

For each tributary, files containing inflows [QTRFN], inflow temperatures [TTRFN], and, if constituents are modeled, then concentrations [CTRFN] must be supplied to the model. If constituents are modeled, the user can select which constituents are included in the tributary concentrations input file (see **Tributary Active Constituent Control** card, page C76).

The user must ensure the number of tributaries parameter [NTP] in the PARAMETER statement in the file W2_INC.FOR is *greater than or equal* to the number of tributaries [NTR] specified on this card (Chapter 3, see page 21).

Example

```
N TRIBS      NTR
              8
```

Related cards and files

Tributary Segment, page C37
Tributary Active Constituent Control, page C76
Tributary Inflow File, page C155
Tributary Temperature File, page C156
Tributary Concentration File, page C157

Tributary Inflow Placement (TRIB PLACE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TRC	Character	Specification of tributary inflows

This card specifies how tributary inflows are distributed into the model layers. There are three options. Inflows can be distributed evenly from top to bottom ([TRC] = DISTR), placed according to density ([TRC] = DENSITY), or the user may specify a range of layer elevations in which the tributary inflows are distributed evenly ([TRC] = SPECIFY). This is similar to the branch inflows, but the additional option allowing the user to specify the range of layer elevations in which to distribute the inflows. This option is particularly usefull when trying to model discharges from a pipe such as wastewater treatment effluent.

If there are *more* tributaries than can be specified on one line, then they are continued on the next line without another **TRIB PLACE** card being specified.

Example

```
TRIB PLACE   TRC      TRC     TRC     TRC     TRC     TRC     TRC     TRC        TRC
             DENSITY   DISTR SPECIFY DENSITY DENSITY DENSITY DENSITY DENSITY
```

Related cards and files

Number of Tributaries, page C35
Tributary Inflow Calculations, page C36
Tributary Segment, page C37
Tributary Inflow Top Elevation, page C38
Tributary Inflow Bottom Elevation, page C39
Tributary Active Constituent Control, page C76
Tributary Inflow File, page C155
Tributary Temperature File, page C156
Tributary Concentration File, page C157

Tributary Segment (TRIB SEG)

Field	Name	Value	Description
1			(Ignored by code)
2-10	ITR	Integer	Segment tributary enters

This card specifies the segment which the tributary enters. Tributary flows are either placed into a layer whose density most closely corresponds to that of the tributary flows, are evenly distributed from top to bottom, or are specified to enter over a range of elevations (see [TRC] on page C36). Flows which enter segments upstream of the current upstream segment [CUS] for a branch are combined with the branch inflow.

If there are **more** tributary segments than can be specified on one line, then they are continued on the next line without another **TRIB SEG** card being specified.

Example

```
TRIB SEG   ITR    ITR    ITR    ITR    ITR    ITR    ITR    ITR    ITR
            2      3      4      3      4      5      6      7
```

Related cards and files

Number of Tributaries, page C35
Tributary Inflow Calculations, page C36
Tributary Inflow Top Elevation, page C38
Tributary Inflow Bottom Elevation, page C39
Tributary Active Constituent Control, page C76
Tributary Inflow File, page C155
Tributary Temperature File, page C156
Tributary Concentration File, page C157

Tributary Inflow Top Elevation (TRIB TOP)

Field	Name	Value	Description
1			(Ignored by code)
2-10	ELTRT	Real	Tributary inflow top elevation, *m above msl*

This card specifies the upper elevation for each tributary inflow in which the user has specified that inflows will be placed over a range of elevations. Only tributaries which are specified as SPECIFY on the **TRIB TOP** card need top elevations specified on this card.

If there are **more** tributary top elevations than can be specified on one line, then they are continued on the next line without another **TRIB TOP** card being specified.

Example

```
TRIB TOP   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT
                           116.0
```

Related cards and files

Number of Tributaries, page C35
Tributary Inflow Calculations, page C36
Tributary Segment, page C37
Tributary Inflow Bottom Elevation, page C39
Tributary Active Constituent Control, page C76
Tributary Inflow File, page C155
Tributary Temperature File, page C156
Tributary Concentration File, page C157

Tributary Inflow Bottom Elevation (ELEV BOT)

Field	Name	Value	Description
1			(Ignored by code)
2-10	ELTRB	Real	*Tributary inflow bottom elevation, m above msl*

This card specifies the bottom elevation for each tributary inflow in which the user has specified that inflows will be placed over a range of elevations. Only tributaries which are specified as SPECIFY on the **TRIB CALC** card need bottom elevations specified on this card.

If there are **more** tributary bottom elevations than can be specified on one line, then they are continued on the next line without another **TRIB BOT** card being specified.

Example

```
TRIB BOT   ELTRB    ELTRB    ELTRB    ELTRB    ELTRB    ELTRB    ELTRB    ELTRB    ELTRB
                             114.0
```

Related cards and files

Number of Tributaries, page C35
Tributary Inflow Calculations, page C36
Tributary Segment, page C37
Tributary Inflow Top Elevation, page C38
Tributary Active Constituent Control, page C76
Tributary Inflow File, page C155
Tributary Temperature File, page C156
Tributary Concentration File, page C157

Distributed Tributaries (DST TRIB)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	DTRC	Character	OFF	Distributed tributary option

This card specifies whether or not a branch contains a distributed tributary. A distributed tributary is equivalent to a non-point source loading. This option may be turned ON or OFF for each branch and is useful in accounting for ungaged flows for the water budget. The flow is distributed among the segments in each branch proportional to their surface areas. There is one value of [DTRC] for each branch.

For each distributed tributary specified, the user must supply an inflow file [QDTFN], an inflow temperature file [TDTFN], and, *if* constituents are modeled, an inflow constituent concentration file [CDTFN].

If constituents are modeled, the user can select which constituents are included in the distributed tributary concentrations input file (see **Distributed Tributary Active Constituent Control** card, page C77).

If there are *more* distributed tributaries than can be specified on one line, then they are continued on the next line without another DST TRIB card being specified.

Example

```
DST TRIB    DTRC    DTRC    DTRC    DTRC    DTRC    DTRC    DTRC    DTRC    DTRC
            OFF     OFF
```

Related cards and files

Distributed Tributary Active Constituent Control, page C77
Distributed Tributary Inflow File, page C158
Distributed Tributary Temperature File, pages C159
Distributed Tributary Concentration File, page C160

Screen Print (SCR PRNT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	SCRC	Character	OFF	Specifies if information is written to the screen
3	NSCR	Integer		Number of screen update intervals

This card specifies if information is output to the screen during the run and the number of intervals during which the frequency of updating the screen can change. The frequency at which the screen is updated should be large (at least 0.1 days). Experience has shown that updating the screen every timestep can easily *double* the runtime.

Example

```
SCR PRNT    SCRC    NSCR
              ON       2
```

Related cards and files

Screen Dates, page C42
Screen Frequency, page C43

Screen Dates (SCR DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SCRD	Real	Dates information is sent to the screen (*Julian day*)

This card specifies the dates information is output to the screen. The total number of dates specified on this card must match [NSCR] on the **Screen Print** card (see page C46).

If there are *more* dates than can be specified on one line, then the values for [SCRD] are continued on the next line without another SCR DATE card being specified.

Example

```
SCR DATE    SCRD    SCRD    SCRD    SCRD    SCRD    SCRD    SCRD    SCRD    SCRD
            224.4   225.5
```

Related cards and files

Screen print, page C41
Screen Frequency, page C43

Screen Frequency (SCR FREQ)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SCRF	Real	Frequency information is sent to the screen, *days*

This card specifies the frequency information is output to the screen. Frequency can be changed at any time during the simulation by specifying appropriate dates on the **Screen Date** card and frequencies on the **Screen Frequency** card.

If there are *more* frequencies than can be specified on one line, then they are continued on the next line without another SCR FREQ card being specified.

Example

```
SCR FREQ   SCRF   SCRF   SCRF   SCRF   SCRF   SCRF   SCRF   SCRF   SCRF
           0.1    1.0
```

Related cards and files

Screen Print, page C41
Screen Dates, page C42

Snapshot Output (SNAPSHOT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	LJPC	Character	OFF	Width of output
3	UPRNC	Character	OFF	Output horizontal velocities
4	WPRNC	Character	OFF	Output vertical velocities
5	TPRNC	Character	OFF	Output temperatures
6	DTPRNC	Character	OFF	Output limiting timestep frequencies

This card specifies the laserjet model and hydrodynamic terms written to the snapshot file [SNPFN]. [LJPC] can be specified as either "OFF", "II", "III", or "IV". The model will output the appropriate codes so that the preprocessor output and snapshot will print on a laserjet compatible hardcopy device. If [LJPC] is set to "OFF", then no codes are output and the user must then have an output device, such as a line printer, that supports 132 column output.

The velocities, temperatures, and limiting timestep frequencies can be turned off in the snapshot file by specifying OFF in the appropriate position on the input card. The printing of constituents is specified in the **Constituent Output** card (see page C74).

Example

```
SNAPSHOT    LJPC    UPRNC    WPRNC    TPRNC
             IV      OFF      OFF       ON
```

Related cards and files

Shortform Segments, page ?
Longform Segments, page C45
Snapshot Print, page C46
Snapshot Dates, page C47
Snapshot Frequency, page C48
Constituent Output, page C74

Snapshot Segments (SNAP SEG)

Field	Name	Value	Description
1			(Ignored by code)
2-10	IPRI	Integer	Segment numbers output to snapshot file
2-9	IPRI	Integer	(continuation)

This card specifies the model segment numbers output to the snapshot file [SNPFN] The user must specify 21 values for [IPRI]. The first nine are entered on the first line. The next nine are entered on the second line and the last three are entered on the third line without another **SNAP SEG** card being specified.

Example

```
SNAP SEG    IPRI    IPRI    IPRI    IPRI    IPRI    IPRI    IPRI    IPRI    IPRI
              2       4       6      10      12      15      17      20      23
             25      27      30      32      34      37      40      42      43
             44      45      46
```

Related cards and files

Snapshot Output, page C44
Snapshot Print, page C46
Snapshot Dates, page C47
Snapshot Frequency, page C48

Snapshot Print (SNP PRNT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	SNPC	Character	OFF	Specifies if information is written to snapshot file
3	NSNP	Integer		Number of snapshot dates

This card specifies if information is output to the snapshot file [SNPFN] and the number of snapshot intervals for specifying output dates and frequencies.

Snapshot file output provides the user with a hard copy of computed values for hydrodynamic and constituent variables for user assigned segments. Output from this file can take up a tremendous amount of disk space and when printed can use up large quantities of computer paper in a short time. This option is generally used during initial runs and then turned off before the user becomes buried in computer output.

The number of snapshot dates [NSNP] refers to the option of writing information to the snapshot file for different dates and frequencies. For example, the user may specify output is to begin on Julian day 224.4 and output every 0.1 days until day 225.5. Information is then output every day until the end of the simulation. In this case, [NSNP] would be set to 2.

Example

```
SNP PRNT    SNPC    NSNP
             ON       2
```

Related cards and files

Snapshot Output, page C44
Shortform Segments, page ?
Longform Segments, page C45
Snapshot Dates, page C47
Snapshot Frequency, page C48

Snapshot Dates (SNP DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SNPD	Real	Dates information is sent to the snapshot file, *Julian day*

This card specifies the dates information is output to the snapshot file [SNPFN]. The total number of dates specified on this card must match [NSNP] on the **Snapshot Print** card (see page C46).

If there are *more* dates than can be specified on one line, then the values for [SNPD] are continued on the next line without another SNP DATE card being specified.

Example

```
SNP DATE    SNPD    SNPD    SNPD    SNPD    SNPD    SNPD    SNPD    SNPD    SNPD
            224.4   225.5
```

Related cards and files

Snapshot Output, page C44
Shortform Segments, page ?
Longform Segments, page C45
Snapshot Print, page C46
Snapshot Frequency, page C48

Snapshot Frequency (SNP FREQ)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SNPF	Real	Frequency information is sent to the snapshot file, *days*

This card specifies the frequency information is output to the snapshot file [SNPFN]. Frequency can be changed at any time during the simulation by specifying appropriate dates on the **Snapshot Date** card and frequencies on the **Snapshot Frequency** card.

If there are **more** frequencies than can be specified on one line, then they are continued on the next line without another SNP FREQ card being specified.

Example

```
SNP FREQ    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF
            0.1     1.0
```

Related cards and files

Snapshot Output, page C44
Shortform Segments, page ?
Longform Segments, page C45
Snapshot Print, page C46
Snapshot Dates, page C47

Profile Plot (PRF PLOT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	PRFC	Character	OFF	Specifies if information is written to the profile file
3	NPRF	Integer	-	Number of profile dates
4	NIPRF	Integer	-	Number of segments to be included in output

This card specifies if information is output to the profile output file [PRFFN], the number of profile intervals for specifying output dates and frequencies, and the number of segments included in the output.

The profile file [PRFFN] is used to plot vertical profiles of temperature and constituents at a specified model segment. This option is normally turned off during initial runs while the user is verifying the model is performing correctly. It is turned on to compare observed data with simulated data during calibration runs.

This file is in a form suitable for FORTRAN postprocessing. The spreadsheet output file can be used for processing output data in a spreadsheet (see page C53).

The **Constituent Output** card (see page C74) controls which constituents are output to the profile file. Temperature is always output to the profile file.

Example

```
PRF PLOT    PRFC    NPRF    NIPRF
            ON      4       12
```

Related cards and files

Profile Dates, page C50
Profile Frequency, page C51
Profile Segment, page C52
Constituent Output, page C74

Profile Dates (PRF DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	PRFD	Real	Dates information is written to the profile file, *Julian day*

This card specifies the dates information is output to the profile file [PRFFN]. If there are **more** dates than can be specified on one line, then they are continued on the next line without another PRF DATE card being specified.

Example

PRF DATE	PRFD	PRFD	PRFD	PRFD	PRFD	PRFD	PRFD	PRFD	PRFD
	100.5	117.5	118.5	224.5					

Related cards and files

Profile Plot, page C49
Profile Frequency, page C51
Profile Segment, page C52
Constituent Output, page C74

Profile Frequency (PRF FREQ)

Field	Name	Value	Description
1			(Ignored by code)
2-10	PRFF	Real	Frequency information is sent to the profile file, *days*

This card specifies the frequency information is output to the profile file [PRFFN]. Frequency can be changed at any time during the simulation by specifying appropriate dates on the **Profile Date** card and frequencies on the **Profile Frequency** card.

If there are **more** frequencies than can be specified on one line, then they are continued on the next line without another PRF FREQ card being specified.

Example

```
PRF FREQ    PRFF    PRFF    PRFF    PRFF    PRFF    PRFF    PRFF    PRFF    PRFF
           100.0     1.0    14.0   100.0
```

Related cards and files

Profile Plot, page C49
Profile Dates, page C50
Profile Segment, page C52
Constituent Output, page C74

Profile Segment (PRF SEG)

Field	Name	Value	Description
1			(Ignored by code)
2-10	IPRF	Real	Segments for which information is written to the profile file

This card specifies model segments for which information is output to the profile file [PRFFN]. If there are *more* segments than can be specified on one line, then they are continued on the next line without another PRF SEG card being specified.

Example

```
PRF SEG    IPRF    IPRF    IPRF    IPRF    IPRF    IPRF    IPRF    IPRF    IPRF
             2       4       6       8      10      14      16      18      20
            23      25      27
```

Related cards and files

Profile Plot, page C49
Profile Dates, page C50
Profile Frequency, page C51
Constituent Output, page C74

Spreadsheet Plot (SPR PLOT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	SPRC	Character	OFF	Specifies if information is written to the spreadsheet file
3	NSPR	Integer	-	Number of spreadsheet dates
4	NISPR	Integer	-	Number of segments to be included in output

This card specifies if information is output to the spreadsheet output file [SPRFN], the number of intervals for specifying output dates and frequencies, and the number of segments included in the output.

The spreadsheet file [SPRFN] is used to plot vertical profiles of temperature and constituents at a specified model segment and is suitable as ASCII input into a spreadsheet type database. This option is normally turned off during initial runs while the user is verifying the model is performing correctly. It is turned on to compare observed data with simulated data during calibration.

The **Constituent Output** card (see page C74) controls which constituents are output to the spreadsheet file. Temperature is always output to the spreadsheet file.

Example

```
SPR PLOT    SPRC    NSPR    NISPR
             ON       4       12
```

Related cards and files

Spreadsheet Dates, page C54
Spreadsheet Frequency, page C55
Spreadsheet Segment, page C56
Constituent Output, page C74

Spreadsheet Dates (SPR DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SPRD	Real	Dates information is written to the spreadsheet file, *Julian day*

This card specifies the dates information is output to the spreadsheet file [SPRFN]. If there are **more** dates than can be specified on one line, then they are continued on the next line without another PRF DATE card being specified.

Example

```
SPR DATE   SPRD     SPRD     SPRD     SPRD     SPRD     SPRD     SPRD     SPRD     SPRD
           100.5    117.5    118.5    224.5
```

Related cards and files

Spreadsheet Plot, page C53
Spreadsheet Frequency, page C55
Spreadsheet Segment, page C56
Constituent Output, page C74

Spreadsheet Frequency (SPR FREQ)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SPRF	Real	Frequency information is sent to the spreadsheet file, *days*

This card specifies the frequency information is output to the spreadsheet file [SPRFN]. Frequency can be changed at any time during the simulation by specifying appropriate dates on the **Spreadsheet Date** card and frequencies on the **Spreadsheet Frequency** card.

If there are **more** frequencies than can be specified on one line, then they are continued on the next line without another PRF FREQ card being specified.

Example

```
SPR FREQ    SPRF    SPRF    SPRF    SPRF    SPRF    SPRF    SPRF    SPRF    SPRF
           100.0     1.0    14.0   100.0
```

Related cards and files

Spreadsheet Plot, page C53
Spreadsheet Dates, page C54
Spreadsheet Segment, page C56
Constituent Output, page C74

Spreadsheet Segment (SPR SEG)

Field	Name	Value	Description
1			(Ignored by code)
2-10	ISPR	Real	Segments for which information is written to the spreadsheet file

This card specifies model segments for which information is output to the spreadsheet file [SPRFN]. If there are *more* segments than can be specified on one line, then they are continued on the next line without another SPR SEG card being specified.

Example

SPR SEG	ISPR	ISPR	ISPR	ISPR	ISPR	ISPR	ISPR	ISPR	ISPR
	2	4	6	8	10	14	16	18	20
	23	25	27						

Related cards and files

Spreadsheet Plot, page C53
Spreadsheet Dates, page C54
Spreadsheet Frequency, page C55
Constituent Output, page C74

Time Series Plot (TSR PLOT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	TSRC	Character	OFF	Specifies if information is written to time series file
3	NTSR	Integer		Number of time series dates

This card specifies if information is output to the times series file [TSRFN] and the number of time series intervals for specifying output dates and frequencies.

The present code outputs information in a form suitable for FORTRAN post-processing. Version 3.0 will include the option to output data in a form suitable for spreadsheet processing.

Example

```
TSR PLOT     TRSC    NTSR
               ON       2
```

Related cards and files

Time Series Dates, page C58
Time Series Frequency, page C59
Constituent Output, page C74

Time Series Dates (TSR DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TSRD	Real	Date information is written to the time series file, *Julian day*

This card specifies the dates information is output to the time series file [TSRFN]. If there are **more** dates than can be specified on one line, then they are continued on the next line without another TSR DATE card being specified.

Example

```
TSR DATE    TSRD    TSRD    TSRD    TSRD    TSRD    TSRD    TSRD    TSRD    TSRD
            224.5   225.5
```

Related cards and files

Time Series Plot, page C57
Time Series Frequency, page C59
Constituent Output, page C74

Time Series Frequency (TSR FREQ)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TSRF	Real	Frequency information is written to the time series file, *days*

This card specifies the frequency information is output to the time series file [TSRFN]. Frequency can be changed at any time during the simulation by specifying the dates on the **Time Series Dates** card and the frequencies on the **Time Series Frequency** card.

If there are **more** frequencies than can be specified on one line, then they are continued on the next line without another TSR FREQ card being specified.

Example

```
TSR FREQ    TSRF    TSRF    TSRF    TSRF    TSRF    TSRF    TSRF    TSRF    TSRF
            0.1     1.0
```

Related cards and files

Time Series Plot, page C57
Time Series Dates, page C58
Constituent Output, page C74

Vector Plot (VPL PLOT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	VPLC	Character	OFF	Specifies if information is written to the vector file
3	NVPL	Integer	-	Number of vector plot dates

This card specifies if information is output to the vector plot file [VPLFN] and the number of vector plot intervals for specifying output dates and frequencies. Version 2.0 requires the user to develop his own means of postprocessing data for vector plots. Version 3.0 will include an X-windows postprocessor capable of producing vector plots.

Example

```
VPL PLOT    VPLC    NVPL
             ON       7
```

Related cards and files

Vector Plot Dates, page C61
Vector Plot Frequency, page C62

Vector Plot Dates (VPL DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	VPLD	Real	Dates information is written to the vector plot file, *Julian day*

This card specifies the dates information is output to the vector plot file [VPLFN]. If there are **more** dates than can be specified on one line, then they are continued on the next line without another VPL DATE card being specified.

Example

VPL DATE	VPLD	VPLD	VPLD	VPLD	VPLD	VPLD	VPLD	VPLD	VPLD
	224.5	225.5	226.5	227.5	228.5	229.5	230.5		

Related cards and files

Vector Plot, page C60
Vector Plot Frequency, page C62

Vector Plot Frequency (VPL FREQ)

Field	Name	Value	Description
1			(Ignored by code)
2-10	VPLF	Real	Frequency information is output to the vector plot file, *days*

This card specifies the frequency information is output to the vector plot file [VPLFN]. Frequency can be changed at any time during the simulation by specifying the dates on the **Vector Plot Date** card and the frequencies on the **Vector Plot Frequency** card.

If there are *more* frequencies than can be specified on one line, then they are continued on the next line without another VPL FREQ card being specified.

Example

```
VPL FREQ    VPLF    VPLF    VPLF    VPLF    VPLF    VPLF    VPLF    VPLF    VPLF
            100.0   100.0   100.0   100.0   100.0   100.0   100.0   100.0   100.0
            100.0   100.0
```

Related cards and files

Vector Plot, page C60
Vector Plot Dates, page C61

Contour Plot (CPL PLOT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	CPLC	Character	OFF	Specifies if information is output to the contour file
3	NCPL	Integer	-	Number of contour plot dates

This card specifies if information is output to the contour plot file [CPLFN] and the number of contour plot intervals for specifying output dates and frequencies. Version 2.0 requires the user to develop his own means of postprocessing data for contour plots. Version 3.0 will include an X-windows postprocessor capable of producing contour plots.

Example

```
CPL PLOT     CPLC     NCPL
               ON        7
```

Related cards and files

Contour Plot Dates, page C64
Contour Plot Frequency, page C65

Contour Plot Dates (CPL DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CPLD	Real	Dates information is output to the contour plot file, *Julian day*

This card specifies the dates information is output to the contour plot file [CPLFN]. If there are *more* dates than can be specified on one line, then they are continued on the next line without another CPL DATE card being specified.

Example

```
CPL DATE   CPLD    CPLD    CPLD    CPLD    CPLD    CPLD    CPLD    CPLD   CPLD
           224.5   225.5   226.5   227.5   228.5   229.5   230.5
```

Related cards and files

Contour Plot, page C63
Contour Plot Frequency, page C65

Contour Plot Frequency (CPL FREQ)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CPLF	Real	Frequency information is output to the contour plot file, *days*

This card specifies the frequency information is output to the contour plot file [CPLFN]. Frequency can be changed at any time during the simulation by specifying appropriate dates on the **Contour Plot Date** card and frequencies on the **Contour Plot Frequency** card.

If there are *more* frequencies than can be specified on one line, then they are continued on the next line without another CPL FREQ card being specified.

Example

```
CPL FREQ   CPLF   CPLF   CPLF   CPLF   CPLF   CPLF   CPLF   CPLF   CPLF
           10.0   10.0   10.0   10.0   10.0   10.0   10.0
```

Related cards and files

Contour Plot, page C63
Contour Plot Dates, page C64

Restart (RESTART)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	RSOC	Character	OFF	Specifies if information is output to the restart file
3	NRSO	Integer	-	Number of restart dates
4	RSIC	Character	OFF	Specifies if information is input from the restart file

This card specifies if information is output to the restart output file [RSOFN] or read into the model from a previously output restart file [RSIFN] and the number of restart dates.

Example

```
RESTART     RSOC     NRSO     RSIC
              ON        2      OFF
```

Related cards and files

Restart Dates, page C67
Restart Frequency, page C68

Restart Dates (RSO DATE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	RSOD	Real	Date information is output to the restart file, *Julian day*

This card specifies dates information is output to the restart file [RSOFN]. If there are *more* dates than can be specified on one line, then they are continued on the next line without another RSO DATE card being specified.

Example

```
RSO DATE    RSOD    RSOD    RSOD    RSOD    RSOD    RSOD    RSOD    RSOD    RSOD
            224.5   230.5
```

Related cards and files

Restart, page C66
Restart Frequency, page C68

Restart Frequency (RSO FREQ)

Field	Name	Value	Description
1			(Ignored by code)
2-10	RSOF	Real	Frequency information is sent to the restart plot file, *days*

This card specifies the frequency information is output to the restart plot file [RSOFN]. Frequencys can be changed at any time during the simulation by specifying the appropriate dates on the **Restart Plot Date** card and frequencies on the **Restart Plot Frequency** card.

If there are *more* frequencies than can be specified on one line, then they are continued on the next line without another RSO FREQ card being specified.

Example

```
RSO FREQ    RSOF     RSOF    RSOF    RSOF    RSOF    RSOF    RSOF    RSOF    RSOF
            100.0    100.0
```

Related cards and files

Restart, page C66
Restart Dates, page C67

Constituent Computations (CST COMP)

Field	Name	Value	Default	Description
1				(Ignored by code)
2	CCC	Character	OFF	Specifies if constituents are computed
3	SDC	Character	OFF	Shift sediment demand during layer addition/subtraction
4	LIMC	Character	OFF	Output algal limiting growth factor
5	KFREQU	Integer	-	Frequency which constituent kinetics are updated

This card starts the specification of constituent computations. [CCC] determines if constituent computations are performed. If this variable is turned off, then constituent computations are not performed and all information specified on the remaining constituent control cards is ignored. Individual constituent computations are controlled on the **Active Constituents** card (see page C71). During the initial calibration runs for freshwater systems, constituent computations are usually turned off until temperature, water surface elevations, and velocities are calibrated.

The [SDC] variable specifies whether longitudinally varying sediment oxygen demand is adjusted upstream or downstream when segments are added or subtracted. This applies only to the zero-order oxygen demand specified on the **Sediment Oxygen Demand** card (see page C93). Oxygen demand exerted by the accumulation of algae and detritus in the sediment compartment is not affected.

The model calculates the limiting factor affecting algal growth - either nitrogen, phosphorus, or light. [LIMC] specifies if the limiting factor is output to the snapshot file.

The model allows the user to update constituent kinetics at a different frequency than constituent transport. The variable [FREQUK] specifies how many transport iterations are performed before constituent kinetics are updated. This option is included primarily to reduce computation time. This variable should initially be set to one during initial calibration. If computation time is of concern, [KFREQU] can be increased until water quality results begin to deviate significantly.

Example

```
CST COMP    CCC    SDC   LIMC  KFREQU
            ON     OFF    ON       1
```

Related cards and files

Active Constituents, page C71
Constituent Initial Concentration, page C73
Constituent Output, page C74
Inflow Active Constituent Control, page C75
Tributary Active Constituent Control, page C76
Distributed Tributary Active Constituent Control, page C77
Precipitation Active Constituent Control, page C78

Active Constituents (CST ACT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	ACC	Character	OFF	Specifies if calculations are to be performed for this constituent
2-10	ACC	Character	OFF	(continuation)
2-4	ACC	Character	OFF	(continuation)

This card specifies which constituents are included in water quality calculations. The following table gives the correspondence between constituents, their number assigned in the model, and input field for the **Active Constituents** card.

Table C-1. Constituent numbers and corresponding input field

Level	Constituent	Constituent number	Input field
I	Tracer	1	2
	Inorganic suspended solids	2	3
	Coliform bacteria	3	4
II	Total dissolved solids	4	5
	Labile DOM	5	6
	Refractory DOM	6	7
	Algae	7	8
	Detritus	8	9
	Phosphate	9	10
	Ammonium	10	2
	Nitrate-nitrite	11	3
	Dissolved oxygen	12	4
	Sediment	13	5
	Total inorganic carbon	14	6
III	Alkalinity	15	7
	pH	16	8
	Carbon dioxide	17	9
	Bicarbonate	18	10
	Carbonate	19	2
IV	Iron	20	3
	CBOD	21	4

If alkalinity calculations are included, then carbon dioxide, bicarbonate, carbonate, and pH are *always* calculated even if the user specifies they not be included.

The user must be certain of what he is doing if he leaves out one or more constituents in level **II**. For example, total inorganic carbon must be simulated to determine the remaining constituents in level **III**. However, total inorganic

carbon is also a function of constituents in level **II**. As stated previously, the constituent kinetics are strongly coupled and failure to include one or more constituents can have far reaching effects that are hard to determine.

Example

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

Related cards and files

Constituent Computations, page C69
Constituent Initial Concentration, page C73
Constituent Output, page C74
Inflow Active Constituent Control, page C75
Tributary Active Constituent Control, page C76
Distributed Tributary Active Constituent Control, page C77
Precipitation Active Constituent Control, page C78

Constituent Initial Concentration (CST ICON)

Field	Name	Value	Description
1			(Ignored by code)
2-10	C2I	Real	Initializes entire grid to this concentration, $g\ m^{-3}$, or specifies a vertical and/or longitudinal profile be used to initialize the grid
2-10	C2I	Real	(continuation)
2-4	C2I	Real	(continuation)

This card allows the user to specify an initial concentration for each constituent. The user has three options. Initial concentrations can be specified as either a single value, a single vertical profile which is used to initialize every segment, or a vertical profile for each segment. Refer to page C71 for the variable names and input field correspondence.

Initial condition	[IC2]
Isoconcentration	>0.0
Single vertical profile	-1.0
Vertical profile at each segment	-2.0

Example

```
CST ICON    C2I      C2I      C2I      C2I      C2I      C2I      C2I      C2I      C2I
            0.0      2.0     10.0     51.0    0.867    2.022     -1.0   0.6667    0.001
          0.002     0.14     -2.0      0.0    11.91     31.0      0.0      0.0      0.0
            0.0      0.1      0.1
```

Related cards and files

Constituent Computations, page C69
Active Constituents, page C71
Vertical Profile File, page C174
Longitudinal Profile File, page C176

Constituent Output (CST PRNT)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	CPRNC	Character	OFF	Specifies if a constituent is printed to files
2-10	CPRNC	Character	OFF	(continuation)
2-4	CPRNC	Character	OFF	(continuation)

This card specifies which constituents are printed to the snapshot file [SNPFN], time series file [TSRFN], profile file [PRFFN], and contour plot file [CPLFN]. The user does not have control over which constituents will be sent to an *individual* file. Refer to page C71 for the variable names and input field correspondence.

Example

```
CST PRNT    CPRNC    CPRNC    CPRNC    CPRNC    CPRNC    CPRNC    CPRNC    CPRNC    CPRNC
              ON      OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF
             OFF      OFF       ON      OFF      OFF      OFF      OFF      OFF      OFF
             OFF      OFF      OFF
```

Related cards and files

Snapshot Print, page C46
Profile Plot, page C49
Time Series Plot, page C57
Contour Plot, page C63

Inflow Active Constituent Control (CIN CON)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	INACC	Character	OFF	Specifies which constituents are included in the inflow constituent file
2-10	INACC	Character	OFF	(continuation)
2-4	INACC	Character	OFF	(continuation)

For some applications, inflow concentrations for a particular constituent may not be available. This card allows the user to include in the inflow concentration file [CINFN] only those constituents for which there is a concentration. Refer to page C71 for the variable names and input field correspondence.

Example

```
CIN CON   INACC   INACC   INACC   INACC   INACC   INACC   INACC   INACC   INACC
           ON      OFF     OFF     OFF     OFF     OFF     OFF     OFF     OFF
           OFF     OFF     ON      OFF     OFF     OFF     OFF     OFF     OFF
           OFF     OFF     OFF
```

Related cards and files

Branch Inflow Constituent File, page C152

Tributary Active Constituent Control (CTR CON)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	TRACC	Character	OFF	Specifies which constituents are included in the tributary inflow constituent file
2-10	TRACC	Character	OFF	(continuation)
2-4	TRACC	Character	OFF	(continuation)

For some applications, tributary inflow concentrations for a particular constituent may not be available. This card allows the user to include in the tributary inflow concentration file [CTRFN] only those constituents for which there is a concentration. Refer to page C71 for the variable names and input field correspondence.

Example

```
CTR CON    TRACC    TRACC    TRACC    TRACC    TRACC    TRACC    TRACC    TRACC    TRACC
           OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF
           OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF
           OFF   .  OFF      OFF
```

Related cards and files

Tributary Inflow Concentration Filename, page C117

Distributed Trib Active Constituent (CDT CON)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	DTACC	Character	OFF	Specifies which constituents are included in the distributed tributary inflow constituent file
2-10	DTACC	Character	OFF	(continuation)
2-4	DTACC	Character	OFF	(continuation)

For some applications, distributed tributary inflow concentrations for a particular constituent may not be available. This card allows the user to include in the distributed tributary inflow concentration file [CDTFN] only those constituents for which there is a concentration. Refer to page C71 for the variable names and input field correspondence.

Example

```
CDT CON   DTACC   DTACC   DTACC   DTACC   DTACC   DTACC   DTACC   DTACC   DTACC
           OFF     OFF     OFF     OFF     OFF     OFF     OFF     OFF     OFF
           OFF     OFF     OFF     OFF     OFF     OFF     OFF     OFF     OFF
           OFF     OFF     OFF
```

Related cards and files

Distributed Tributary Inflow Concentration File, page C160

Precipitation Active Constituent Control (CPR CON)

Field	Name	Value	Default	Description
1				(Ignored by code)
2-10	PRACC	Character	OFF	Specifies which constituents are included in the precipitation inflow constituent file
2-10	PRACC	Character	OFF	(continuation)
2-4	PRACC	Character	OFF	(continuation)

For some applications, precipitation concentrations for a particular constituent may not be available. This card allows the user to include in the precipitation concentration file [CPRFN] only those constituents for which there is a concentration. Refer to page C71 for the variable names and input field correspondence.

Example

```
CPR CON    PRACC    PRACC    PRACC    PRACC    PRACC    PRACC    PRACC    PRACC    PRACC
           OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF
           OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF      OFF
           OFF      OFF      OFF
```

Related cards and files

Calculations, page C12

Extinction Coefficients (EX COEF)

Field	Name	Value	Description
1			(Ignored by code)
2	EXH2O	Real	Extinction for water, m^{-1}
3	EXINOR	Real	Extinction due to inorganic suspended solids, $m^3\ m^{-1}\ g^{-1}$
4	EXORG	Real	Extinction due to organic suspended solids, $m^3\ m^{-1}\ g^{-1}$
5	BETA	Real	Fraction of incident solar radiation absorbed at the water surface

This card specifies the extinction coefficients and amount of solar radiation, β, absorbed in the surface layer. Extinction coefficients are used to calculate a net extinction coefficient, γ, which is determined from the following equation:

$$\gamma = \epsilon_{H_2O} + \epsilon_{iss}\Phi_{iss} + \epsilon_{oss}\Phi_{oss} \qquad \text{(B-54)}$$

where:

γ = net extinction coefficient

ϵ_{H2O} = light extinction exclusive of suspended solids

ϵ_{iss} = light extinction due to inorganic suspended solids

ϵ_{oss} = light extinction due to organic suspended solids (algae + detritus)

Φ_{iss} = inorganic suspended solids concentration, $g\ m^{-3}$

Φ_{oss} = organic suspended solids (algae + detritus) concentration, $g\ m^{-3}$

ϵ_{H2O} varies greatly depending upon the dissolved substances in the water. Table 4, Table C-2 gives values reported in the literature which can be used as rudimentary guidelines for selecting a value of ϵ_{H2O}.

Megard et al. (1980) and Smith and Baker (1978) determined each gram per cubic meter of chlorophyll increased ϵ_{oss} by 22 and 16 m^{-1}, respectively. Averaging the two values and assuming a carbon to algal biomass ratio of 0.45 and a carbon to chlorophyll ratio of 50, then each gram per cubic meter of algal biomass should increase ϵ_{oss} by about 0.17 m^{-1}. However, the carbon to chlorophyll ratios vary from 25 to 150. Values for ϵ_{iss} should be of the same order of magnitude as ϵ_{oss}.

If any constituents included in equation (B-54) are not included in the simulation, then the value for ϵ_{H2O} should be increased to account for the constituent left out. Equation (B-55) can be used to estimate the extinction coefficient.

Table C-2. Literature Values for Extinction Coefficient.

Location	Description	γ, m^{-1}	Reference
Lake Tahoe, CA	Oligotrophic	0.2	Wetzel, 1975
Crystal Lake, WI	Oligotrophic	0.2	Wetzel, 1975
Crater Lake, OR	Oligotrophic	0.18	Spence, 1981
Lake Borralie, Scotland	Calcareous water	0.34	Spence, 1981
Wintergreen Lake, MI	Eutrophic	0.46-1.68	Wetzel, 1975
Lake Paajarvi, Finland	Brown-stained	0.7	Verduin, 1982
Loch Unagan, Scotland	Brown-stained	1.53	Spence, 1981
Loch Leven, Scotland	Turbid, eutrophic	2.58	Spence, 1981
Neusiedlersee, Austria	Turbid	3.31	Spence, 1981
Highly stained lakes	Average	4.0	Wetzel, 1975

$$\gamma = 1.11 \, Z_s^{-0.73} \qquad\qquad (B\text{-}55)$$

where

γ = net extinction coefficient

Z_s = secchi disk depth, m

Equation (B-55) includes the effects of ϵ_{iss} and ϵ_{oss} and should be used only when inorganic and organic suspended solids are not included in the simulation.

The fraction of incident solar radiation absorbed at the water surface, β, represents solar radiation absorbed in a 0.6 m surface layer. Once γ has been determined, Equation (B-56) can be used to determine β.

$$\beta = 0.27 \ln(\gamma) + 0.61 \qquad\qquad (B\text{-}56)$$

Example

```
EX COEF    EXH2O   EXINOR   EXORG   BETA
            0.45    0.10     0.17    0.45
```

Coliform (COLIFORM)

Field	Name	Value	Description
1			(Ignored by code)
2	COLQ10	Real	Coliform Q_{10} coefficient
3	COLDK	Real	Coliform decay rate, day^{-1}

This card specifies the Q_{10} coefficient and decay rate for coliform. The model uses a Q_{10} formulation to modify the coliform decay rate as a function of temperature. The Q_{10} coefficient is usually 1.04. A range of values can be found in Zison et al. (1978).

Coliform decay rate is a function of sedimentation, solar radiation, nutrient availability, predation, algae, bacterial toxins, and physicochemical factors. For studies in which bacterial contamination is of important concern, efforts should be made to obtain *in situ* decay rate measurements. Methods for obtaining decay rates can be found in Frost and Streeter (1924), Marais (1974), and Zison et al. (1978). Table C-3 gives reported literature values for coliform decay rates.

Table C-3. *In Situ* Coliform Decay Rates

Location	Season/Temperature	Rate, day^{-1}	Reference
Ohio River	Summer, 20 °C	1.18	Frost and Streeter, 1924
Ohio River	Winter, 5 °C	1.08	Frost and Streeter, 1924
Upper Illinois River	June-September	2.04	Hoskins, et al, 1927
Upper Illinois River	October-May	2.52, 0.89	Hoskins, et al, 1927
Upper Illinois River	December-March	0.57, 0.62	Hoskins, et al, 1927
Upper Illinois River	April-November	1.03, 0.70	Hoskins, et al, 1927
Missouri River	Winter	0.48	Kittrell and Furfari, 1963
Tennessee River	Summer	1.03, 1.32	Kittrell and Furfari, 1963
Tennessee River	Summer	1.32	Kittrell and Furfari, 1963
Sacramento River	Summer	1.75	Kittrell and Furfari, 1963
Cumberland River	Summer	5.52	Kittrell and Furfari, 1963
Leaf River, MS	-	0.41	Mahloch, 1974
Wastewater lagoon	7.0-25.5 °C	0.20-0.70	Klock, 1971
Maturation ponds	19 °C	1.68	Marais, 1974
Oxidation ponds	20 °C	2.59	Marais, 1974

Example

```
COLIFORM  COLQ10   COLDK
            1.04     1.1
```

Suspended Solids (S SOLIDS)

Field	Name	Value	Description
1			(Ignored by code)
2	SSETL	Real	Suspended solids settling rate, $m\ day^{-1}$

This card specifies the suspended solids settling rate. Settling rate is a function of particle type, grain size, density, viscosity, and turbulence. The model uses a net settling velocity which does not explicitly account for these factors and it is up to the user to choose an appropriate value. For waterbodies with high suspended sediment loads, selection of appropriate values for the settling velocity is critical for a successful application. For most large waterbodies, the larger particles settle very quickly and should not be included in the inflow. Lane (1938) gives values of 0.86 to 860.0 $m\ day^{-1}$ for particle diameters of 0.002 to 0.1 mm. Particles found in the main body of a reservoir are usually at the lower end of this range.

Example

```
S SOLIDS   SSETL
             2.0
```

Algae (ALGAE)

Field	Name	Value	Description
1			(Ignored by code)
2	AGROW	Real	Algal growth rate, day^{-1}
3	AMORT	Real	Algal mortality rate, day^{-1}
4	AEXCR	Real	Algal excretion rate, day^{-1}
5	ARESP	Real	Algal dark respiration rate, day^{-1}
6	ALGS	Real	Algal settling rate, day^{-1}
7	ASAT	Real	Saturation intensity at maximum photosynthetic rate, $W\,m^{-2}$
8	APOM	Real	Fraction of algal biomass lost by mortality to detritus

This card specifies rates for algal growth, mortality, excretion, respiration, and settling, fraction of algal biomass lost by mortality to detritus, and algal light saturation intensity at maximum photosynthetic rate.

[AGROW] is the maximum gross production rate which is not corrected for respiration, mortality, excretion, or sinking. Most literature values report net production rates which take into account respiration so care must be taken when using reported literature values. The user must evaluate the experimental design to determine if reported values represent gross or net production rates. Also, [AGROW] is temperature dependent. If the expected temperature in the photic zone is 25°C, then the user should select rates measured near this temperature.

Maximum algal mortality rate [AMORT] is also temperature dependent. A general rule of thumb is [AMORT] should be less than 10% of [AGROW]. Values ranging from 0.01 to 0.03 have been used in previous modeling studies.

[AEXCR] is the maximum algal excretion (or photorespiration) rate which goes directly to the labile DOM compartment. Literature values are reported in Table C-4.

Table C-4. Literature values for maximum algal excretion rates

Species	Excretion Rate, day^{-1}	Reference
Actinastrum hantzschii	0.044	Nalewajko, 1966
Ankistrodesmus falcatus	0.031	Nalewajko, 1966
Asterococcus superbus	0.036	Nalewajko, 1966
Chlorella pyrenoidosa	0.032	Nalewajko, 1966
Eudorina elegans	0.023	Nalewajko, 1966
Micractinium pusillum	0.014	Nalewajko, 1966

[ARESP] is the maximum dark algal respiration rate. Respiration rates are often expressed as millilitres of oxygen consumed per milligram of organism dry weight per hour. To convert to model units (mg O_2 mg^{-1} organism dry weight day^{-1}), multiply dark respiration rates by 0.74 mg dry weight/1 ml O_2. Table C-5 gives literature values for respiration rates.

Table C-5. Literature values for algal dark respiration rates

Species	Respiration Rate, day^{-1}	Reference
Anabaena variabilis	0.10-0.92	Collins and Boylen, 1978
Chlorella pyrenoidosa	0.01-0.03	Myers and Graham, 1961
Coscinodiscus excentricus	0.07-0.11	Riley and von Aux, 1949
Dunaliella teriolecta	0.12-0.16	Laws and Wong, 1978
Mesodinium rubrum	0.05	Smith, 1979
Monochrysis lutheri	0.15-0.32	Laws and Wong, 1978
Thalassiosira allenii	0.05-0.59	Laws and Wong, 1978

[ALGS] is a representative settling velocity for algal assemblages. Literature values are given in table C-6, but care must be taken in their use. Laboratory and *in situ* methods for determining settling velocities each have their drawbacks when attempting to measure net settling velocities.

Table C-6. Literature values for algal settling velocities

Species	Settling velocity, $m\ day^{-1}$	Reference
Diatoms		
Asterionella formosa	0.26-0.76	Smayda, 1974
Bacteriastrum hyalinum	0.39-1.27	Smayda & Boleyn, 1966
Chaetoceros didymus	0.85	Eppley Holmes, & Strickland, 1967b
Chaetoceros lauderi	0.46-1.54	Smayda & Boleyn, 1966
Chaetoceros spp.	0.85	Margalef, 1961
Chaetoceros spp.	4.00	Allen, 1932

Species	Settling velocity, $m\ day^{-1}$	Reference
Coscinodiscus wailesii	7.00-30.2	Eppley Holmes, & Strickland, 1967b
Coscinodiscus sp.	1.95-6.83	Eppley Holmes, & Strickland, 1967b
Cyclotella meneghiniana	0.08-0.24	Titman & Kilham, 1976
Cyclotella nana	0.16-0.76	Eppley Holmes, & Strickland, 1967b
Ditylum brightwellii	0.60-3.09	Eppley Holmes, & Strickland, 1967b
Fragilaria crotonensis	0.27	Burns & Rosa, 1980
Leptocylindrum danicus	0.08-0.42	Margalef, 1961
Melosira agassizii	0.67-1.87	Titman & Kilham, 1976
Nitzschia closterium	0.52	Margalef, 1961
Nitzschia seriata	0.35-0.50	Smayda & Boleyn, 1965
Phaeodactylum tricornutu	0.02-0.06	Riley, 1943
Rhizosolenia hebetata	0.22	Eppley, Holmes, & Strickland, 1967b
Rhizosolenia setigera	0.10-6.30	Smayda & Boleyn, 1974
Rhizosolenia stolterfothii	1.00-1.9	Eppley, Holmes, & Strickland, 1967b
Rhizosoleni sp.	0.00-0.72	Margalef, 1961
Skeletonema costatum	0.30-1.35	Smayda & Boleyn, 1974
Stephanopyxis turris	1.10	Eppley, Holmes, & Strickland, 1967b
Thalassionema nitzsiodes	0.35-0.78	Smayda (unpublished)
Thalassiosira fluviatilis	0.60-1.10	Eppley, Holmes, & Strickland, 1967b
Thalassiosira nana	0.10-0.28	Smayda & Boleyn, 1966
Thalassiosira rotula	0.39-2.10	Smayda & Boleyn, 1966
Dinoflagellates		
Gonyaulax polyedra	2.80-6.10	Bramlette, 1961
Coccolithophorids		
Coccolithus huxleyi	0.28, 1.2	Eppley, Holmes, & Strickland, 1967b
Cricosphaera carterae	1.7	Eppley, Holmes, & Strickland, 1967b
Cricosphaera elongata	0.25	Eppley, Holmes, & Strickland, 1967b
Cycloccolithus fragilus	10.3-13.2	Bernard, 1963
Microflagellates		
Cryptomonas reosa	0.31	Burns & Rosa, 1980
Cryptomonas marsonii	0.32	Burns & Rosa, 1980
Rhodomonas minuta	0.07	Burns & Rosa, 1980
Monochrysis lutheri	0.39	Eppley, Holmes, & Strickland, 1967b
Greens		
Closterium parvulum	0.18	Burns & Rosa, 1980
Dunaliella tertiolecta	0.18	Eppley, Holmes, & Strickland, 1967b
Lagerhaemia quadriseta	0.08	Burns & Rosa, 1980

Species	. Settling velocity, $m\ day^{-1}$	Reference
Scenedesmus acutiformis	0.10	Burns & Rosa, 1980
Selenastrum minutum	0.15	Burns & Rosa, 1980
Bluegreens		
Anabaena spiroides	0.10	Burns & Rosa, 1980
Gomphosphaeria lacustris	0.11	Burns & Rosa, 1980

[ASAT] is the saturating light intensity at the maximum photosynthetic rate. Since phytoplankton adapt to low light regimes, saturation coefficients may be lower than those measured in the laboratory. Table C-7 gives literature values for [ASAT].

Table C-7. Literature values for saturating light intensity

Species	Saturation, $W\ m^{-2}$	Reference
Cryptomonas ovata	12-36	Cloern, 1977
Oscillatoria agardhii	10	van Lierre, et al., 1978
Oscillatoria rubescens	36-61	Konopka, 1983
Scenedesmus protuberans	24	van Lierre, et al., 1978
Mixed diatoms	86	Belay, 1981
Mixed phytoplankton	36	Belay, 1981
Shade-adapted phytoplankton	18-29	Belay, 1981

[APOM] is the fraction of algal biomass lost by mortality going into the detritus compartment with the remainder going to labile DOM. Otsuki and Hayna (1972) have reported a value of 0.8 for *Scenedesmus* sp.

Example

```
ALGAE    AGROW   AMORT   AEXCR   ARESP   ALGS    ASAT    APOM
         1.1     0.01    0.01    0.02    0.14    150.0   0.8
```

Related cards and files

Algal Rate Coefficients, page C87

Algal Rate Coefficients (ALG RATE)

Field	Name	Value	Description
1			(Ignored by code)
2	ALGT1	Real	Lower temperature for algal growth, $^\circ C$
3	ALGT2	Real	Lower temperature for maximum algal growth, $^\circ C$
4	ALGT3	Real	Upper temperature for maximum algal growth, $^\circ C$
5	ALGT4	Real	Upper temperature for algal growth, $^\circ C$
6	AGK1	Real	Fraction of algal growth rate at ALGT1
7	AGK2	Real	Fraction of maximum algal growth rate at ALGT2
8	AGK3	Real	Fraction of maximum algal growth rate at ALGT3
9	AGK4	Real	Fraction of algal growth rate at ALGT4

This card specifies the lower, maximum lower, upper, and maximum upper temperatures used in defining the curve which determines effects of temperature on algal growth rates. See Appendix B, page B30 for more details on the mathematical formulation for the temperature coefficients.

Example

```
ALG RATE   AGT1    AGT2    AGT3    AGT4    AGK1    AGK2    AGK3    AGK4
           10.0    30.0    35.0    40.0    0.1     0.99    0.99    0.1
```

Related cards and files

Algae, page C83

Dissolved Organic Matter (DOM)

Field	Name	Value	Description
1			(Ignored by code)
2	LDOMDK	Real	Labile DOM decay rate, day^{-1}
3	LRDK	Real	Labile to refractory decay rate, day^{-1}
4	RDOMDK	Real	Maximum refractory decay rate, day^{-1}

This card specifies decay rates associated with dissolved organic matter. Dissolved organic matter in the model is divided into labile and refractory partitions. The labile partition has a higher decay rate and generally consists of autochthonous inputs such as early products of algal decay. Table 8 gives literature values for various organic compounds. The refractory decay rate, [RDOMDK], is generally two orders of magnitude smaller than the labile decay rate [LDOMDK]. If BOD decay rates are available, then they should be used as a starting point for [LDOMDK].

Table C-8. Literature values for labile DOM decay rates

Compound	Decay Rate, day^{-1}	Reference
Acetate	0.20	Wright, 1975
Amino acids	0.64	Williams et al., 1976
Glucose	0.24	Williams et al., 1976
Glucose	0.32-0.50	Toerien and Cavari, 1982
Glucose	0.11	Wright, 1975
Glutamate	0.11-0.63	Carney and Colwell, 1976
Glycine	0.31-0.45	Vaccaro, 1969
Glycolate	0.01-0.43	Wright, 1975

Example

```
DOM      LDOMDK    LRDK   RDOMDK
          0.12     0.001   0.001
```

Particulate Organic Matter (POM)

Field	Name	Value	Description
1			(Ignored by code)
2	LPOMDK	Real	Detritus decay rate, day^{-1}
3	LPOMS	Real	Detritus settling rate, day^{-1}

Detritus in the model consists of autochthonous and allocthonous particulate organic matter (POM). The model uses a single decay rate [LPOMDK], but in reality, detritus is a heterogeneous mixture in varyious stages of decay. Allochthonous inputs are usually refractory while autochthonous inputs are initially labile becoming refractory over time. The present model formulation does not allow for spatially and temporally varying detritus decay rates. Literature values for detritus decay rates are given in Table C-9.

Table C-9. Literature values for detritus decay rates

Detritus Source	Detritus Decay Rate, day^{-1}	Reference
Cladophera glomerata	0.007	Piecznska, 1972
Gloeotrichia echinulata	0.001-0.007	Piecznska, 1972
Isoetes lancustris	0.003-0.015	Hanlon, 1982
Potamogeton crispus	0.002-0.004	Rogers & Breen, 1982
Potamogeton perfoliatus	0.002-0.007	Hanlon, 1982
Beech litter	0.001-0.004	Hanlon, 1982
Green algae	0.016-0.076	Otsuki & Hayna, 1972
Mixed algae	0.007-0.111	Jewell & McCarty, 1971
Mixed algae	0.007-0.060	Fitzgerald, 1964
Leaf packs	0.005-0.017	Sedell, Triska, and Triska, 1975

Detrital settling velocities [LPOMS] vary over a large range (0.001 to > 20 m day^{-1}) depending upon the detritus. Again, the model allows for only a single value. Literature values are given in Table C-10.

Table C-10. Literature values for detritus settling velocities

Detritus Source	Settling Velocity, $m\ day^{-1}$	Reference
Ceratium balticum	9.0	Apstein, 1910
Chaetoceros borealis	9.0	Apstein, 1910
Chaetoceros didymus	0.85	Eppley, Holmes, & Strickland, 1967
Cricosphaera carterae	1.70	Eppley, Holmes, & Strickland, 1967
Ditylum brightwellii	2.0	Apstein, 1910
Phaeodactylum tricornutum	0.02-0.04	Riley, 1943
Rhizosolenia herbetata	0.22	Eppley, Holmes, & Strickland, 1967b
Stephanopyxis tunis	2.1	Eppley, Holmes, & Strickland, 1976b
Tabellaria flocculosa	0.46-1.5	Smayda, 1971
Thalassiosira psuedonana	0.85	Hecky & Kilham, 1974

Example

```
DETRITUS  LPOMDK    LPOMS
          0.06      0.35
```

Related cards and files

Organic Rate Multipliers, page C91

Organic Rate Multipliers (ORG RATE)

Field	Name	Value	Description
1			(Ignored by code)
2	OMT1	Real	Lower temperature for organic matter decay, °C
3	OMT2	Real	Lower temperature for maximum organic matter decay, °C
4	OMK1	Real	Fraction of organic matter decay rate at OMT1
5	OMK2	Real	Fraction of organic matter decay rate at OMT2

This card specifies the lower and maximum lower temperatures used in defining the curve which determines effects of temperature on organic matter decay. See Appendix B, page B30 for more details on the mathematical formulation for the temperature coefficients. Recommended values are given in the example.

Example

```
ORG RATE    OMT1    OMT2   OMK1    OMK2
            4.0     20.0    0.1    0.99
```

Related cards and files

Detritus, page C89

Sediment (SEDIMENT)

Field	Name	Value	Description
1			(Ignored by code)
2	SEDDK	Real	Sediment decay rate, day^{-1}
3	FSOD	Real	Fraction of SOD

This card specifies the sediment decay rate which should be of comparable magnitude as the labile decay rate. If the sediment compartment is included during simulations, then the following equation can be used to compare oxygen consumption rates with reported literature values. [SEDDK] can then be adjusted accordingly.

$$O_{2\ demand} = [SEDDK]\ \Phi_{sed}\ \sigma \qquad (B\text{-}57)$$

where

$O_{2\ demand}$ = oxygen consumption rate at the sediment/water interface, $g\ C\ m^2\ day^{-1}$

Φ_{sed} = value of sediments in the sediment compartment, $g\ m^{-2}$

σ = carbon to oxygen stoichiometric equivalent

The fraction of SOD [FSOD] is used to rapidly adjust the values of [SOD] during calibration. The value for [SOD] is multiplied by [FSOD] at each segment to adjust values.

Example

```
SEDIMENT   SEDDK   FSOD
           0.06    0.9
```

Related cards and files

Sediment Oxygen Demand, page C93

Sediment Oxygen Demand (S DEMAND)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SOD	Real	Sediment oxygen demand for each segment, $g\ C\ m^2\ day^{-1}$

This card specifies the zero-order sediment oxygen demand for each segment (including boundary segments) in the computational grid. If there are *more* values than can be specified on one line, then they are continued on the next line without another S DEMAND card being specified.

Sediment oxygen demand is known to vary spatially in reservoirs due to differences in sedimentation patterns and algal production (Cole & Hannan, 1989). In the model, the user can specify a separate value of [SOD] for each model segment. Sediment oxygen demand typically ranges from 0.1 to 1.0g O_2 m^2 day^{-1} but can be higher (Newbold and Liggett, 1974). Additional information can be found in Gunnison, Chen, and Brannon (1983) and Chen, Brannon, and Gunnison (1984). Additional values are given in Table C-11.

Table C-11. Literature values for sediment oxygen demand

Site	SOD, $g\ C\ m^2\ day^{-1}$	Reference
Cayuga Lake, NY	0.3-1.0	Newbold & Liggett, 1974
Lake Sammamish, WA	1.0	Bella, 1970
Lake Lyndon B. Johnson, TX	1.7-5.8	Schnoor & Fruh, 1979
Saginaw River, MI	0.1-5.3	Chiaro & Burke, 1980

Example

```
S DEMAND   SOD    SOD    SOD    SOD    SOD    SOD    SOD    SOD    SOD
           0.2    0.2    0.2    0.2    0.2    0.2    0.3    0.4    0.5
           0.5    0.5    0.5    0.5    0.5    0.5    0.4    0.4    0.3
           0.3    0.3    0.2    0.2    0.2    0.2    0.2    0.2    0.2
           0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2
           0.2    0.2
```

Related cards and files

Sediment, page C92

Carbonaceous Biochemical Oxygen Demand (CBOD)

Field	Name	Value	Description
1			(Ignored by code)
2	KBOD	Real	5-day decay rate @ 20°C, day^{-1}
3	TBOD	Real	Temperature coefficient
4	RBOD	Real	Ratio of BOD5 to ultimate BOD

BOD has been added to Version 2.0. [KBOD] is the first-order reaction constant. [TBOD] is used to adjust the decay rate for temperature effects according to the following equation:

$$KBOD = KBOD_{20} \times TBOD^{(T-20)}$$

where T is the temperature and $KBOD_{20}$ is the decay rate at 20°C. [RBOD] is used to convert 5-day BOD values to ultimate BOD.

The present formulation accounts only for BOD effects on dissolved oxygen and does not recycle nutrients to the water column. It is intended primarily for applications which involve determining the effects of waste effluents on dissolved oxygen in which loadings are typically expressed in terms of BOD.

Example

```
CBOD        KBOD    TBOD    RBOD
            0.25    1.047   1.85
```

Phosphorus (PHOSPHOR)

Field	Name	Value	Description
1			(Ignored by code)
2	PO4REL	Real	Sediment release rate of phosphorous (fraction of SOD)
3	PARTP	Real	Phosphorous partitioning coefficient for suspended solids
4	AHSP	Real	Algal half-saturation constant for phosphorous, $g\ m^{-1}$

[PO4REL] is the sediment release rate of phosphorous under anaerobic conditions specified as a fraction of the sediment oxygen demand. Values up to 0.3 have been used in previous studies. [PARTP] is the phosphorous partioning coefficient for sorption onto suspended solids. [AHSP] is the algal half-saturation constant for phosphorous and is defined as the phosphorous concentration at which the uptake rate is one-half the maximum rate. This represents the upper concentration at which algal growth is directly proportional to phosphorous concentrations.

Example

```
PHOSPHOR  PO4REL    PARTP    AHSP
          0.015      1.2    0.009
```

Table C-12. Literature values for phosphorus half-saturation constant

Species	Half-Saturation Constant, $mg\ l^{1}$	Reference
Asterionella formosa	0.002	Holm & Armstrong, 1981
Asterionella japonica	0.014	Thomas & Dodson, 1968
Biddulphia sinensis	0.016	Quasim, et al., 1973
Cerataulina bergonii	0.003	Finenko & Krupatkina, 1974
Chaetoceros curvisetus	0.074-0.105	Finenko & Krupatkina, 1974
Chaetoceros socialis	0.001	Finenko & Krupatkina, 1974
Chlorella pyrenoidosa	0.380-0.475	Jeanjean, 1969
Cyclotella nana	0.055	Fuhs, et al., 1972
Cyclotella nana	0.001	Fogg, 1973
Dinobryon cylindricum	0.076	Lehman (unpublished)
Dinobryon sociale	0.047	Lehman (unpublished)
Euglena gracilis	1.520	Dlum, 1966
Microcystis aeruginosa	0.006	Holm & Armstrong, 1981
Nitzschia actinastreoides	0.095	Von Muller, 1972
Pediastrum duplex	0.105	Lehman (unpublished)
Pithophora oedogonia	0.980	Spencer & Lembi, 1981
Scenedesmus obliquus	0.002	Fogg, 1973
Scenedesmus sp.	0.002-0.050	Rhee, 1973
Thalosssiosira fluviatilis	0.163	Fogg, 1973

Ammonia (AMMONIA)

Field	Name	Value	Description
1			(Ignored by code)
2	NH4REL	Real	Sediment release rate of ammonia (fraction of SOD)
3	NH4DK	Real	Ammonia decay rate, day^{-1}
4	PARTN	Real	Ammonia partioning coefficient for suspended solids
5	AHSN	Real	Algal half-saturation constant for ammonia

[NH4REL] is the sediment release rate of ammonia anaerobic conditions specified as a fraction of the sediment oxygen demand. Values up to 0.4 have been used in previous studies.

[NH4DK] is the rate at which ammonia is oxidized to nitrate-nitrite. Since the model considers nitrate-nitrite as one compartment, the rate specified should be the rate for conversion of ammonia to nitrate. Literature values are given in Table C-13.

Table C-13. Literature values for ammonia oxidation rates

Site	Ammonia decay rate, day^{-1}	Reference
Grand River, IL	0.80	Bansal, 1976
Grasmerer Lake, UK	0.001-0.013	Hall, 1982
Truckee River, NV	0.09-1.30	Bansal, 1976
Mohawk River, NY	0.23-0.40	Bansal, 1976
Ohio River	0.25	Bansal, 1976
Big Blue River, NB	0.17-0.25	Bansal, 1976
Flint River, MI	0.76-0.95	Bansal, 1976

[PARTN] is the ammonia partitioning coefficient for sorption onto suspended solids.

[AHSN] is the algal half-saturation constant for nitrogen and is defined as the nitrogen concentration (ammonia + nitrate/nitrite) at which the uptake rate is one-half the maximum rate. This represents the upper concentration at which algal growth is proportional to nitrogen. Table C-14 gives literature values for the nitrogen half-saturation constant.

Table C-14. Literature values for nitrogen half-saturation constant.

Species	Half saturation constant	N source	Reference
Diatoms			
Biddulphia aurita	0.056-0.197	NO3	Underhill, 1977
Chaetoceros gracilis	0.012	NO3	Eppley, Rogers, & McCarthy, 1969
	0.012	NH4	Eppley, Rogers, & McCarthy, 1969
Coscinodiscus lineatus	0.012	NO3	Eppley, Rogers, & McCarthy, 1969
	0.012	NH4	Eppley, Rogers, & McCarthy, 1969
Cyclotella nana	0.025-0.117	NO3	Carpenter & Guillard, 1971
	0.111		MacIsaac & Dugdale, 1969
	0.027		Caperon & Meyer, 1972
	0.031		Eppley, Rogers, & McCarthy, 1969
Ditylum brightwellii	0.037	NO3	Eppley, Rogers, & McCarthy, 1969
	0.020	NO3	Eppley, Rogers, & McCarthy, 1969
Dunaliella teriolecta	0.013	NO3	Caperon & Meyer, 1972
	0.013	NH4	Caperon & Meyer, 1972
	0.087	NO3	Eppley, Rogers, & McCarthy, 1969
Fragilaria pinnata	0.037-0.100	NO3	Carpenter & Guillard, 1971
Leptocylindrous danicus	0.078	NO3	Eppley, Rogers, & McCarthy, 1969
	0.013	NH4	Eppley, Rogers, & McCarthy, 1969
Navicula pelliculosa	0.923	NO3	Wallen & Cartier, 1975
Phaeodactylum tricornutum	0.161	NO3	Ketchum, 1939
Rhizosolenia robusta	0.186	NO3	Eppley, Rogers, & McCarthy, 1969
	0.135	NH4	Eppley, Rogers, & McCarthy, 1969
Rhizosolenia stolterfothii	0.105	NO3	Eppley, Rogers, & McCarthy, 1969
	0.009	NH4	Eppley, Rogers, & McCarthy, 1969
Skeletonema costatum	0.027	NO3	Eppley, Rogers, & McCarthy, 1969
	0.014	NH4	Eppley, Rogers, & McCarthy, 1969
Bluegreens			
Anabaena cylindrica	4.34	NO3	Hattori, 1962
	2.48	NO3	Hattori, 1962
Asterionella formosa	0.074-0.093	NO3	Eppley & Thomas, 1969
	0.062	NH4	Eppley & Thomas, 1969
Oscillatoria agardhii	0.22	NO3	van Lierre, 1977
Microflagellates			
Bellochia sp.	0.001-0.16	NO3	Carpenter & Guillard, 1971
Monochrysis lutheri	0.026	NO3	Caperon & Meyer, 1972
	0.052	NH4	Caperon & Meyer, 1972
	0.037	NO3	Eppley, Rogers, & McCarthy, 1969
	0.007	NH4	Eppley, Rogers, & McCarthy, 1969
Coccolithophorids			

Species	Half saturation constant	N source	Reference
Coccolithus huxleyi	0.006	NO3	Eppley, Rogers, & McCarthy, 1969
	0.002	NH4	Eppley, Rogers, & McCarthy, 1969
Greens			
Chlorella pyrendoidosa	0.006-0.14		Pickett, 1975
	1.15	NO3	Knudsen, 1965
Pithophora cedogonia	1.236	NO3	Spencer & Lembi, 1981
Dinoflagellates			
Gonyaulax polyedra	0.589	NO3	Eppley, Rogers, & McCarthy, 1969
	0.099	NH4	Eppley, Rogers, & McCarthy, 1969
Gymnodinium splendens	0.235	NO3	Eppley, Rogers, & McCarthy, 1969
	0.099	NH4	Eppley, Rogers, & McCarthy, 1969
Gymnodinium wailesii	0.223	NO3	Eppley, Rogers, & McCarthy, 1969
	0.088	NH4	Eppley, Rogers, & McCarthy, 1969
Chrysophytes			
Isochrysis galbana	0.006	NO3	Eppley, Rogers, & McCarthy, 1969

Example

```
AMMONIUM  NH4REL   NH4DK   PARTN    AHSN
           0.08    0.12     1.0    0.014
```

Related cards and files

Ammonia Rate Multipliers, page C100

Ammonia Rate Multipliers (NH4 RATE)

Field	Name	Value	Description
1			(Ignored by code)
2	NH4T1	Real	Lower temperature for ammonia decay, $^{\circ}C$
3	NH4T2	Real	Lower temperature for maximum ammonia decay, $^{\circ}C$
4	NH4K1	Real	Fraction of nitrification rate at NH4T1
5	NH4K2	Real	Fraction of nitrification rate at NH4T2

This card specifies the lower and maximum lower temperatures used in defining the curve which determines the effect of temperature on ammonia nitrification. See Appendix B, page B30 for more details on the mathematical formulation for the temperature coefficients. Recommended values are given in the example.

Example

```
NH4 RATE   NH4T1   NH4T2   NH4K1   NH4K2
            5.0    20.0     0.1    0.99
```

Related cards and files

Ammonia, page C97

Nitrate (NITRATE)

Field	Name	Value	Description
1			(Ignored by code)
2	NO3DK	Real	Nitrate decay rate, *day*$^{-1}$

This card specifies the denitrification rate. Values used in previous modeling studies have ranged from 0.05-0.15 day^{-1}.

Example

```
NITRATE    NO3DK
           0.102
```

Related cards and files

Nitrate Rate Multipliers, page C102

Nitrate Rate Multipliers (NO3 RATE)

Field	Name	Value	Description
1			(Ignored by code)
2	NO3T1	Real	Lower temperature for nitrate decay, $°C$
3	NO3T2	Real	Lower temperature for maximum nitrate decay, $°C$
4	NO3K1	Real	Fraction of denitrification rate at NO3T1
5	NO3K2	Real	Fraction of denitrification rate at NO3T2

This card specifies the lower and maximum lower temperatures used in defining the curve which determines the effect of temperature on denitrification. See Appendix B, page B30 for more details on the mathematical formulation for the temperature coefficients. Recommended values are given in the example.

Example

```
NO3 RATE    NO3T1    NO3T2   NO3K1   NO3K2
              5.0     20.0     0.1     0.99
```

Related cards and files

Nitrate, page C101

Sediment Carbon Dioxide Release (SED CO2)

Field	Name	Value	Description
1			(Ignored by code)
2	CO2REL	Real	Sediment carbon dioxide release rate (fraction of sediment oxygen demand)

This card specifies the carbon dioxide release rate from the sediments as a fraction of sediment oxygen demand.

Example

```
SED CO2   CO2REL
              0.1
```

Related cards and files

Sediment Oxygen Demand, page C93

Iron (IRON)

Field	Name	Value	Description
1			(Ignored by code)
2	FEREL	Real	Iron sediment release rate (fraction of sediment oxygen
3	FESETL	Real	Iron settling velocity, $m\ day^{-1}$

[FEREL] specifies the iron release rate from the sediments as a fraction of the sediment oxygen demand. Values between 0.3 and 0.5 have been used in previous modeling studies.

[FESETL] is the particulate iron settling rate in the water column under oxic conditions. Values between 0.5 and 2.0 have been used in previous modeling studies.

Example

```
IRON      FEREL  FESETL
           0.5    2.0
```

Related cards and files

Sediment Oxygen Demand, page C93

Stoichiometry (STOICHMT)

Field	Name	Value	Description
1			(Ignored by code)
2	O2NH4	Real	Oxygen stoichiometric equivalent for ammonia decay
3	O2ORG	Real	Oxygen stoichiometric equivalent for organic matter decay
4	O2RESP	Real	Oxygen stoichiometric equivalent for dark respiration
5	O2ALG	Real	Oxygen stoichiometric equivalent for algal growth
6	BIOP	Real	Stoichiometric equivalent between organic matter and phosphorous
7	BION	Real	Stoichiometric equivalent between organic matter and nitrogen
8	BIOC	Real	Stoichiometric equivalent between organic matter and carbon

This card specifies the stoichiometric equivalents used in the model. These values should not be changed unless the user has data to support the new value.

Example

```
STOICHMT   O2NH3   O2ORG  O2RESP   O2ALG    BIOP   BION  . BIOC
            4.57     1.4     1.4     1.4   0.011   0.08    0.45
```

Oxygen Limit (O2 LIMIT)

Field	Name	Value	Description
1			(Ignored by code)
2	O2LIM	Real	Dissolved oxygen concentration at which an-aerobic processes begin, $g\ m^{-3}$

This card specifies the dissolved oxygen concentration below which anaerobic processes such as nitrification and sediment nutrient releases take place.

Example

```
O2 LIMIT    O2LIM
               0.2
```

Bathymetry Filename (BTH FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	BTHFN	Character	Bathymetry filename

This card specifies the filename containing the waterbody bathymetry.

Example

```
BTH FILE.........................BTHFN....................................
      bth.npt
```

Vertical Profile Filename (VPR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	VPRFN	Character	Temperature and constituent vertical profile filename used for specifying initial conditions for the grid

This card specifies the filename used to specify vertically varying initial temperatures and concentrations for the grid. See page C174 for more information on data setup.

Example

```
VPR FILE.............................VPRFN.....................................
        vpr.npt
```

Longitudinal Profile Filename (LPR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	LPRFN	Character	Temperature and constituent longitudinal profile filename used for specifying initial conditions for the grid

This card specifies the filename used to specify vertically and longitudinally varying initial temperatures and concentrations for the grid. See page C176 for more information on data setup.

Example

```
LPR FILE..............................LPRFN.....................................
        lpr.npt
```

Restart Input Filename (RSI FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	RSIFN	Character	Restart input data filename

This card specifies the filename used as input for restarts.

Example

```
RSI FILE.............................RSIFN....................................
        rsi.npt
```

Meteorologic Data Filename (MET FILE)

Field **Name** **Value** **Description**
1   (Ignored by code)
2-10   METFN   Character   Meteorologic input data filename

This card specifies the filename for time-varying meteorologic data. See page C149 for more information on data setup.

Example

```
MET FILE...............................METFN....................................
        met.npt
```

Withdrawal Filename (QWD FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	QWDFN	Character	Withdrawal filename

This card specifies the filename for withdrawal outflows. See page C154 for more information on data setup.

Example

```
QWD FILE.............................QWDFN...................................
       qwd.npt
```

Branch Inflow Filename (QIN FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	QINFN	Character	Inflow filename

This card specifies the filename(s) for branch inflows. See page C150 for more information on data setup.

Example

```
QIN FILE......................QINFN....................................
Br 1    qin_br1.npt
Br 2    qin_br2.npt
Br 3    qin_br3.npt
```

Branch Inflow Temperature Filename (TIN FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TINFN	Character	Inflow temperature filename

This card specifies the filename(s) for branch inflow temperatures. See page
C151 for more information on data setup.

Example

```
TIN FILE...........................TINFN.....................................
Br 1    tin_br1.npt
Br 2    tin_br2.npt
Br 3    tin_br3.npt
```

Branch Inflow Constituent Filename (CIN FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CINFN	Character	Inflow constituent filename

This card specifies the filename(s) for branch inflow concentrations. See page C152 for more information on data setup.

Example

```
CIN FILE........................CINFN...............................
Br 1    cin_br1.npt
Br 2    cin_br2.npt
Br 3    cin_br3.npt
```

Branch Outflow Filename (QOT FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	QOTFN	Character	Outflow filename

This card specifies the filename(s) for branch outflows. See page C153 for more information on data setup.

Example

```
QOT FILE..............................QOTFN.....................................
Br 1    qot_br1.npt
Br 2    qot_br2.npt
```

Tributary Inflow Filename (QTR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	QTRFN	Character	Tributary inflow filename

This card specifies the filename(s) for tributary inflows. There must be a separate file for *each* tributary. See page C155 for more information on data setup.

Example

```
QTR FILE...........................QTRFN.................................
Tr 1    qtr_tr1.npt
Tr 2    qtr_tr2.npt
```

Tributary Inflow Temperature Filename (TTR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TTRFN	Character	Tributary temperature filename

This card specifies the filename(s) for tributary inflow temperatures. There must be a separate file for *each* tributary. See page C156 for more information on data setup.

Example

```
TTR FILE.............................TTRFN.....................................
Tr 1    ttr_tr1.npt
Tr 2    ttr_tr2.npt
```

Tributary Inflow Concentration Filename (CTR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CTRFN	Character	Tributary inflow concentration filename

This card specifies the filename(s) for tributary inflow concentrations. There must be a separate file for *each* tributary. See page C157 for more information on data setup.

Example

```
CTR FILE.......................CTRFN....................................
Tr 1    ctr_tr1.npt
Tr 2    ctr_tr2.npt
```

Distributed Tributary Inflow Filename (QDT FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	QDTFN	Character	Distributed tributary inflow filename

This card specifies the filename(s) for distributed tributary inflow. There must be a separate file for *each* branch. See page C158 for more information on data setup.

Example

```
QDT FILE...............................QDTFN.....................................
Br 1    qdt_tr1.npt
Br 2    qdt_tr2.npt
```

Distributed Tributary Inflow Temperature
Filename (TDT FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TDTFN	Character	Distributed tributary temperature filename

This card specifies the filename(s) for distributed tributary inflow temperatures. There must be a separate file for **each** branch. See page C159 for more information on data setup.

Example

```
TDT FILE..............................TDTFN....................................
Br 1    tdt_tr1.npt
Br 2    tdt_tr2.npt
```

Distributed Tributary Inflow Concentration Filename (CDT FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CDTFN	Character	Distributed tributary inflow concentration file-name

This card specifies the filename(s) for distributed tributary inflow concentrations. There must be a separate file for **each** branch. See page C160 for more information on data setup.

Example

```
CDT FILE...............................CDTFN....................................
Br 1    cdt_tr1.npt
Br 2    cdt_tr2.npt
```

Precipitation Filename (PRE FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	PREFN	Character	Precipitation filename

This card specifies the filename(s) for each branch precipitation. There must be a separate file for *each* branch. See page C161 for more information on data setup.

Example

```
PRE FILE.............................PREFN....................................
Br 1    pre_br1.npt
Br 2    pre_br2.npt
```

Precipitation Temperature Filename (TPR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TPRFN	Character	Precipitation temperature filename

This card specifies the filename(s) for branch precipitation temperatures. There must be a separate file for *each* branch. See page C162 for more information on data setup.

Example

```
TPR FILE.............................TPRFN.................................
Br 1    tpr_br1.npt
Br 2    tpr_br2.npt
```

Precipitation Concentration Filename (CPR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CPRFN	Character	Precipitation concentration filename

This card specifies the filename(s) for branch precipitation constituent concentrations. There must be a separate file for *each* branch. See page C163 for more information on data setup.

Example

```
CPR FILE...............................CPRFN..................................
Br 1    cpr_br1.npt
Br 2    cpr_br2.npt
```

External Upstream Head Filename (EUH FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	EUHFN	Character	External upstream head filename

This card specifies the filename(s) for branch external upstream heads. There must be a separate file for *each* branch. See page C164 for more information on data setup.

Example

```
EUH FILE..............................EUHFN.....................................
Br 1    euh_br1.npt
Br 2    euh_br2.npt
```

External Upstream Head Temperature Filename
(TUH FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TUHFN	Character	External upstream head temperature filename

This card specifies the filename(s) for branch external upstream head vertical temperatures. There must be a separate file for *each* branch. See page C165 for more information on data setup.

Example

```
TUH FILE..............................TUHFN.....................................
Br 1    tuh_br1.npt
Br 2    tuh_br2.npt
```

External Upstream Head Concentration Filename (CUH FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CUHFN	Character	External upstream head concentration filename

This card specifies the filename(s) for branch external upstream head constituent concentrations. There must be a separate file for *each* branch. See page C167 for more information on data setup.

Example

```
CUH FILE.............................CUHFN.....................................
Br 1    cuh_br1.npt
Br 2    cuh_br1.npt
```

External Downstream Head Filename (EDH FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	EDHFN	Character	External downstream head filename

This card specifies the filename(s) for branch external downstream heads. There must be a separate file for *each* branch. See page C169 for more information on data setup.

Example

```
EDH FILE.............................EDHFN....................................
Br 1    edh_br1.npt
Br 2    edh_br2.npt
```

External Downstream Head Temperature Filename (TDH FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TDHFN	Character	External downstream head temperature file-name

This card specifies the filename(s) for branch external downstream head vertical temperatures. There must be a separate file for **each** branch. See page C170 for more information on data setup.

Example

```
TDH FILE.............................TDHFN.....................................
Br 1    tdh_br1.npt
Br 2    tdh_br2.npt
```

External Downstream Head Concentration
Filename (CDH FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CDHFN	Character	External downstream had concentration file-name

This card specifies the filename(s) for branch external downstream head constituent concentrations. There must be a separate file for *each* branch. See page C172 for more information on data setup.

Example

```
CDH FILE...........................CDHFN.....................................
Br 1    cdh_br1.npt
Br 2    cdh_br2.npt
```

Snapshot Filename (SNP FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SNPFN	Character	Snapshot filename

This card specifies the snapshot filename.

Example

```
SNP FILE..............................SNPFN....................................
         snp.opt
```

Restart Output Filename (RSO FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	RSOFN	Character	Restart output filename

This card specifies the restart output filename.

Example

```
RSO FILE...........................RSOFN.....................................
        rso.opt
```

Time Series Plot Filename (TSR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	TSRFN	Character	Time series plot filename

This card specifies the time series plot filename.

Example

```
TSR FILE.........................TSRFN.................................
        tsr.opt
```

Profile Plot Filename (PRF FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	PRFFN	Character	Profile plot filename

This card specifies the vertical profile plot filename.

Example

```
PRF FILE...........................PRFFN...................................
        prf.opt
```

Vector Plot Filename (VPL FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	VPLFN	Character	Vector plot filename

This card specifies the velocity vector plot filename.

Example

```
VPL FILE.............................VPLFN....................................
        vpl.opt
```

Contour Plot Filename (CPL FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	CPLFN	Character	Contour plot filename

This card specifies the contour plot filename.

Example

```
CPL FILE.............................CPLFN.....................................
          cpl.opt
```

Spreadsheet Plot Filename (SPR FILE)

Field	Name	Value	Description
1			(Ignored by code)
2-10	SPRFN	Character	Spreadsheet plot filename

This card specifies the spreadsheet output filename. Output from this file is suitable for import into a spreadsheet or graphics package which uses a spreadsheet format for data management.

Example

```
SPR FILE..............................SPRFN...................................
       spr.opt
```

Sample Control Input File

Degray Lake control file for CE-QUAL-W2

```
TITLE C ..........................TITLE...................................
        Degray Reservoir, March 5 through December 24, 1980
        Density placed inflows, point sink outflow
        AX=1, DX=1, CHEZY=70, CBHE=7e-8, TSED=13, WSC=0.85
        Station @ dam
        Temperature and water quality simulation
        Run 1

TIME CON  TMSTRT   TMEND    YEAR
           63.5    357.7    1980

DLT CON      NDT  MINDLT
              1     1.0

DLT DATE    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD
            63.5

DLT MAX   DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX
          7200.0

DLT FRN     DLTF    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF
            0.90

BRANCH G      US      DS     UHS     DHS
               2      31       0       0

LOCATION     LAT    LONG   ELBOT
            34.2    93.3   66.35

INIT CND     T2I  ICETHI  WTYPEC
            -1.0     0.0   FRESH

CALCULAT     VBC     EBC     MBC     PQC    PQTC     EVC     PRC
              ON      ON      ON      ON     OFF     OFF     OFF

INTERPOL   INFIC    TRIC   DTRIC    HDIC   OUTIC    WDIC   METIC
              ON     OFF     OFF     OFF      ON     OFF      ON

DEAD SEA   WINDC    QINC   QOUTC   HEATC
              ON      ON      ON      ON

ICE COVER   ICEC   SLICEC   SLHTC  ALBEDO     HWI   BETAI  GAMMAI  ICEMIN   ICET2
             OFF   DETAIL    TERM    0.25    10.0     0.6    0.07    0.05     3.0

TRANSPORT  SLTRC   THETA
         QUICKEST    0.55

WSC NUMB    NWSC
               1

WSC DATE    WSCD    WSCD    WSCD    WSCD    WSCD    WSCD    WSCD    WSCD    WSCD
            63.5

WSC COEF     WSC     WSC     WSC     WSC     WSC     WSC     WSC     WSC     WSC
            0.85
```

HYD COEF	AX	DX	CHEZY	CBHE	TSED				
	1.0	1.0	75.0	7.0E-8	13.0				
SEL WITH	SWC	SWC	SWC	SWC	SWC	SWC	SWC	SWC	SWC
	ON								
N STRUC	NSTR	NSTR	NSTR	NSTR	NSTR	NSTR	NSTR	NSTR	NSTR
	1								
K BOTTOM Br 1	KBSW	KBSW	KBSW	KBSW	KBSW	KBSW	KBSW	KBSW	KBSW
	35								
SINK TYPE Br 1	SINKC	SINKC	SINKC	SINKC	SINKC	SINKC	SINKC	SINKC	SINKC
	POINT								
E STRUC Br 1	ESTR	ESTR	ESTR	ESTR	ESTR	ESTR	ESTR	ESTR	ESTR
	114.0								
W STRUC Br 1	WSTR	WSTR	WSTR	WSTR	WSTR	WSTR	WSTR	WSTR	WSTR
N OUTLET	NOUT	NOUT	NOUT	NOUT	NOUT	NOUT	NOUT	NOUT	NOUT
	0								
O LAYER Br 1	KOUT	KOUT	KOUT	KOUT	KOUT	KOUT	KOUT	KOUT	KOUT
N WDRWAL	NWD								
	0								
W SEGMNT	IWD	IWD	IWD	IWD	IWD	IWD	IWD	IWD	IWD
W LAYER	KWD	KWD	KWD	KWD	KWD	KWD	KWD	KWD	KWD
N TRIBS	NTR	NTR	NTR	NTR	NTR	NTR	NTR	NTR	NTR
	0								
TRIB SEG	ITR	ITR	ITR	ITR	ITR	ITR	ITR	ITR	ITR
DST TRIB	DTRC	DTRC	DTRC	DTRC	DTRC	DTRC	DTRC	DTRC	DTRC
	OFF								
SNAPSHOT	LJPC	UPRNC	WPRNC	TPRNC	DTPRNC				
	IV	OFF	OFF	ON	ON				
SNAP SEG	IPRI	IPRI	IPRI	IPRI	IPRI	IPRI	IPRI	IPRI	IPRI
	2	4	7	10	12	13	14	15	18
	19	20	22	23	24	25	26	27	28
	29	30	31						
SNP PRNT	SNPC	NSNP							
	ON	22							
SNP DATE	SNPD	SNPD	SNPD	SNPD	SNPD	SNPD	SNPD	SNPD	SNPD
	63.5	77.7	91.7	105.7	119.7	135.7	147.7	161.7	175.7
	189.7	203.7	217.7	231.7	245.7	259.7	273.7	287.7	301.7
	315.7	329.7	343.7	357.7					

SNP FREQ	SNPF	SNPF	SNPF	SNPF	SNPF	SNPF	SNPF	SNPF	SNPF
	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
	100.0	100.0	100.0	100.0					

PRF PLOT	PRFC	NPRF	NIPRF
	ON	22	3

PRF DATE	PRFD	PRFD	PRFD	PRFD	PRFD	PRFD	PRFD	PRFD	PRFD
	63.7	77.7	91.7	105.7	119.7	135.7	147.7	161.7	175.7
	189.7	203.7	217.7	231.7	245.7	259.7	273.7	287.7	301.7
	315.7	329.7	343.7	357.7					

PRF FREQ	PRFF	PRFF	PRFF	PRFF	PRFF	PRFF	PRFF	PRFF	PRFF
	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
	100.0	100.0	100.0	100.0					

PRF SEG	IPRF	IPRF	IPRF	IPRF	IPRF	IPRF	IPRF	IPRF	IPRF
	10	18	26						

TSR PLOT	TSRC	NTSR
	OFF	0

TSR DATE	TSRD	TSRD	TSRD	TSRD	TSRD	TSRD	TSRD	TSRD	TSRD

TSR FREQ	TSRF	TSRF	TSRF	TSRF	TSRF	TSRF	TSRF	TSRF	TSRF

VPL PLOT	VPLC	NVPL
	OFF	0

VPL DATE	VPLD	VPLD	VPLD	VPLD	VPLD	VPLD	VPLD	VPLD	VPLD

VPL FREQ	VPLF	VPLF	VPLF	VPLF	VPLF	VPLF	VPLF	VPLF	VPLF

CPL PLOT	CPLC	NCPL
	OFF	0

CPL DATE	CPLD	CPLD	CPLD	CPLD	CPLD	CPLD	CPLD	CPLD	CPLD

CPL FREQ	CPLF	CPLF	CPLF	CPLF	CPLF	CPLF	CPLF	CPLF	CPLF

RESTART	RSOC	NRSO	RSIC
	OFF	0	OFF

RSO DATE	RSOD	RSOD	RSOD	RSOD	RSOD	RSOD	RSOD	RSOD	RSOD

RSO FREQ	RSOF	RSOF	RSOF	RSOF	RSOF	RSOF	RSOF	RSOF	RSOF

CST COMP	CCC	LIMC	SDC	KFREQU
	ON	ON	OFF	6

CONTROL FILE

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

CST ICON	IC2	IC2	IC2	IC2	IC2	IC2	IC2	IC2	IC2
	0.0	2.0	10.0	51.0	0.7	2.022	-1.0	0.1	0.001
	0.002	0.14	-1.0	-2.0	11.91	31.0	0.0	0.0	0.0
	0.0	0.1	0.0						

CST PRNT	CPRN	CPRN	CPRN	CPRN	CPRN	CPRN	CPRN	CPRN	CPRN
	OFF	ON	OFF	ON	ON	ON	ON	ON	ON
	ON	ON	ON	ON	OFF	OFF	OFF	OFF	OFF
	OFF	OFF	OFF						

CIN CON	INACC	INACC	INACC	INACC	INACC	INACC	INACC	INACC	INACC
	ON	ON	ON	ON	ON	ON	ON	ON	ON
	ON	ON	ON	ON	ON	ON	ON	OFF	OFF
	OFF	ON	OFF						

CTR CON	TRACC	TRACC	TRACC	TRACC	TRACC	TRACC	TRACC	TRACC	TRACC
	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF
	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF
	OFF	OFF	OFF						

CDT CON	DTACC	DTACC	DTACC	DTACC	DTACC	DTACC	DTACC	DTACC	DTACC
	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF
	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF
	OFF	OFF	OFF						

CPR CON	PRACC	PRACC	PRACC	PRACC	PRACC	PRACC	PRACC	PRACC	PRACC
	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF
	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF	OFF
	OFF	OFF	OFF						

EX COEF	EXH2O	EXINOR	EXORG	BETA
	0.45	0.01	0.4	0.45

COLIFORM	COLQ10	COLDK
	1.04	1.4

S SOLIDS	SSETL
	2.0

ALGAE	AGROW	AMORT	AEXCR	ARESP	ALGS	ASAT	APOM
	2.05	0.10	0.06	0.06	0.10	75.0	0.80

ALG RATE	AGT1	AGT2	AGT3	AGT4	AGK1	AGK2	AGK3	AGK4
	5.0	30.0	35.0	40.0	0.1	0.99	0.99	0.1

DOM	LDOMDK	LRDK	RDOMDK
	0.20	0.010	0.001

POM	LPOMDK	LPOMS
	0.08	0.10

ORG RATE	OMT1	OMT2	OMK1	OMK2
	5.0	25.0	0.1	0.99

SEDIMENT	SEDDK	FSOD
	0.08	1.0

S DEMAND	SOD	SOD	SOD	SOD	SOD	SOD	SOD	SOD	SOD
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0				

CBOD	KBOD	TBOD	RBOD
	0.25	1.0147	1.85

PHOSPHOR	PO4REL	PARTP	AHSP
	0.015	1.2	0.006

AMMONIUM	NH4REL	NH4DK	PARTN	AHSN
	0.08	0.12	1.0	0.014

NH4 RATE	NH4T1	NH4T2	NH4K1	NH4K2
	5.0	30.0	0.1	0.99

NITRATE	NO3DK
	0.12

NO3 RATE	NO3T1	NO3T2	NO3K1	NO3K2
	5.0	30.0	0.1	0.99

SED CO2	CO2REL
	0.1

IRON	FEREL	FESETL
	0.5	2.0

STOICHMT	O2NH4	O2ORG	O2RESP	O2ALG	BIOP	BION	BIOC
	4.57	1.4	1.4	1.4	0.011	0.08	0.45

O2 LIMIT	O2LIM
	0.00

```
BTH FILE...............................BTHFN.................................
        bth.npt

VPR FILE...............................VPRFN.................................
        vpr.npt

LPR FILE...............................LPRFN.................................
        lpr.npt

RSI FILE...............................RSIFN.................................
        rsi.npt - not used

MET FILE...............................METFN.................................
        met.npt

QWD FILE...............................QWDFN.................................
        qwd.npt - not used

QIN FILE...............................QINFN.................................
Br 1    qin_br1.npt

TIN FILE...............................TINFN.................................
Br 1    tin_br1.npt

CIN FILE...............................CINFN.................................
Br 1    cin_br1.npt
```

```
QOT FILE..............................QOTFN.....................................
Br 1    qot_br1.npt

QTR FILE..............................QTRFN.....................................
Tr 1    qtr_tr1.npt - not used

TTR FILE..............................TTRFN.....................................
Tr 1    ttr_tr1.npt - not used

CTR FILE..............................CTRFN.....................................
Tr 1    ctr_tr1.npt - not used

QDT FILE..............................QDTFN.....................................
Tr 1    qdt_br1.npt - not used

TDT FILE..............................TDTFN.....................................
Tr 1    tdt_br1.npt - not used

CDT FILE..............................CDTFN.....................................
Tr 1    cdt_br1.npt - not used

PRE FILE..............................PREFN.....................................
Br 1    pre_br1.npt - not used

TPR FILE..............................TPRFN.....................................
Br 1    tpr_br1.npt - not used

CPR FILE..............................CPRFN.....................................
Br 1    cpr_br1.npt - not used

EUH FILE..............................EUHFN.....................................
Br 1    euh_br1.npt - not used

TUH FILE..............................TUHFN.....................................
Br 1    tuh_br1.npt - not used

CUH FILE..............................CUHFN.....................................
Br 1    cuh_br1.npt - not used

EDH FILE..............................EDHFN.....................................
Br 1    edh_br1.npt - not used

TDH FILE..............................TDHFN.....................................
Br 1    tdh_br1.npt - not used

CDH FILE..............................CDHFN.....................................
Br 1    cdh_br1.npt - not used

SNP FILE..............................SNPFN.....................................
        snp.opt

TSR FILE..............................TSRFN.....................................
        tsr.opt

PRF FILE..............................PRFFN.....................................
        prf.opt

VPL FILE..............................VPLFN.....................................
        vpl.opt

CPL FILE..............................CPLFN.....................................
        cpl.opt
```

```
SPR FILE................................SPRFN..................................
        spr.opt
```

Bathymetry File

The bathymetry file contains information specifying the segment lengths, water surface elevations, segment orientations, layer heights, and average widths for each grid cell. The following is a list of guidelines for file preparation.

1. The first three lines are ignored and can be used to comment the input file.
2. Segment lengths, water surface elevations, segment orientations, layer heights, and cell widths at each segment are preceded by two lines which are ignored. They can be used to comment each individual segment's bathymetry.
3. Input format for each cell width is F8.0 with 10 cell widths per line.
4. It is recommended the user number the branches starting with the mainstem as branch 1. The remaining branch numbers should be numbered consecutively starting with the most upstream branch followed by the remaining branches as one moves downstream.
5. Each branch is surrounded by a segment of boundary cells (cells with zero widths) on both the upstream and downstream ends. Note this requirement results in *two segments* of zero widths between each branch.
6. Boundary cells must also be included at the top and bottom of each segment.
7. If there are *more* cell widths than can fit on one line, then they are continued immediately on the next line.
8. The number of segments must agree with the value of [IMP] in the file W2.INC
9. Cell widths start at layer 1 and continue to the maximum number of layers [KMP] The number of layers specified in this file must match the value of [KMP] in the file W2.INC.
10. Only cells that are potentially active have non-zero widths. The first layer, boundary segment cells, and cells below the reservoir bottom elevation at a given segment have zero widths.

The following bathymetry file gives an example for a three branch case involving a mainstem and two branches for a total number of 20 segments [IMP] and 22 layers [KMP].

Example

```
     CE-QUAL-W2 sample bathymetry file - 3 branches, [IMP]=20, [KMP]=22

Segment lengths [DLX]
   1000.0  1000.0  1000.0  1000.0   900.0  1000.0   900.0   800.0   900.0   900.0
    500.0   500.0   500.0   500.0   500.0   500.0   500.0   500.0   500.0   500.0

Water surface elevation [ELWS]
    123.8   123.8   123.8   123.8   123.8   123.8   123.8   123.8   123.8    0.10
    123.8   123.8   123.8   123.8   123.8   123.8   123.8   123.8   123.8    0.10

Segment orientations [PHIO]
      2.5     2.5     2.5     2.5     2.5     2.5     2.5     2.5     2.5     2.5
      3.5     3.5     3.5     3.5     3.5     3.5     0.5     0.5     0.5     0.5

Layer heights [H]
      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     1.0     1.0     1.0     1.0     1.0
      1.0     1.0

Segment 1 - branch 1 upstream boundary
      0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
      0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
      0.      0.

Segment 2 - branch 1
      0.    315.    285.    255.    225.    195.    175.    135.    128.    123.
    120.    115.    108.    100.     93.     60.      0.      0.      0.      0.
      0.      0.

Segment 3 - branch 1
      0.    315.    285.    255.    225.    195.    175.    135.    128.    123.
    120.    115.    108.    100.     60.      0.      0.      0.      0.      0.
      0.      0.

Segment 4 - branch 1
      0.   1661.   1496.   1331.   1166.   1001.   1001.    671.    618.    534.
    390.    155.     61.     50.      0.      0.      0.      0.      0.      0.
      0.      0.

Segment 5 - branch 1
      0.   1392.   1392.   1392.   1385.   1369.   1234.   1148.    917.    636.
    486.    268.    100.      0.      0.      0.      0.      0.      0.      0.
      0.      0.

Segment 6 - branch 1
      0.   1221.   1196.   1171.   1146.   1121.   1096.   1086.   1071.   1022.
    972.    932.    833.    680.    506.    367.      0.      0.      0.      0.
      0.      0.

Segment 7 - branch 1
      0.    489.    481.    472.    464.    455.    450.    438.    429.    383.
    331.    305.    258.    241.    160.    139.    116.    110.     99.      0.
      0.      0.

Segment 8 - branch 1
      0.   1253.   1232.   1211.   1190.   1169.   1148.   1136.   1133.   1103.
    969.    900.    783.    667.    535.    326.    111.     81.     69.     54.
     46.      0.
```

```
Segment 9 - branch 1
     0.   1711.   1690.   1669.   1648.   1627.   1606.   1585.   1564.   1548.
  1542.   1539.   1536.   1326.    915.    729.    637.    414.    185.    167.
   136.      0.

Segment 10 - branch 1 downstream boundary
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.

Segment 11 - branch 2 upstream boundary
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.

Segment 12 - branch 2
     0.     53.     52.     51.     50.     49.     49.     47.     39.     25.
    18.     10.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.

Segment 13 - branch 2
     0.    180.    171.    166.    142.    125.    114.     98.     96.     95.
    94.     90.     76.     51.     12.      0.      0.      0.      0.      0.
     0.      0.

Segment 14 - branch 2
     0.    426.    417.    408.    399.    390.    386.    373.    336.    316.
   306.    300.    293.    266.    193.    137.     20.      0.      0.      0.
     0.      0.

Segment 15 - branch 2
     0.    326.    324.    322.    320.    318.    318.    312.    306.    297.
   294.    285.    273.    256.    241.    191.    144.     24.      0.      0.
     0.      0.

Segment 16 - branch 2 downstream boundary
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.

Segment 17 - branch 3 upstream boundary
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.

Segment 18 - branch 3
     0.    342.    342.    342.    342.    342.    342.    342.    299.    226.
   168.    142.     75.     73.     70.     64.     61.     49.     35.     26.
    20.      0.

Segment 19 - branch 3
     0.    467.    460.    453.    446.    439.    436.    425.    414.    288.
   256.    180.    144.     65.     61.     58.     58.     50.     47.     47.
    43.      0.

Segment 20 - branch 3 downstream boundary
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
     0.      0.
```

Meteorologic File

The meteorologic input file contains the following data:

Variable Description	Name	Format
Julian date	[JDAY]	F8.0
Air temperature, °C	[TAIR]	F8.0
Dewpoint temperature, °C	[TDEW]	F8.0
Wind speed, $m\ sec^{-1}$	[WIND]	F8.0
Wind direction, rad	[PHI]	F8.0
Cloud cover	[CLOUD]	F8.0

The following is a list of guidelines for file preparation:

1. Data is read in according to an F8.0 format which allows the user to override the decimal point location according to the location specified in the input file. The field widths *must* be the same as specified above.
2. The first two lines are ignored and can be used to comment the file.
3. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
4. Data can be input at any frequency and may vary during the simulation. The user need only specify the Julian date corresponding to the data.

Example

```
Sample meteorologic input file

  JDAY    TAIR    TDEW    WIND     PHI   CLOUD
   1.0     7.8    -0.9    2.19     2.0     8.0
   2.0     3.3     1.3    4.75     2.0     6.0
   3.0     3.3     1.3    4.75     2.0     3.0
   4.0     2.2    -3.5    3.33     2.0     4.0
   5.0     6.4    -2.4    1.86     2.0     4.0
   6.0     7.5     2.4    4.00     2.0    10.0
   7.0     1.9    -4.9    4.83     2.0     2.0
   8.0     1.7    -6.6    4.00     2.0     0.0
```

Branch Inflow File

This file contains the inflow for a branch with an upstream flow boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch with an upstream flow boundary condition (see page C8). This allows the user to update inflows for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The second field is the inflow rate, $m^3 \ sec^{-1}$.

Note the following example takes advantage of the algorithm's capability to use data at varying frequencies.

Example

```
CE-QUAL-W2 sample inflow file

     JDAY      QIN
182.0000      0.
182.5416    283.
182.6250    566.
182.6666   1699.
182.7916    566.
182.8333    283.
182.9166      0.
185.5416    283.
185.6250    566.
185.6666   1699.
185.7916    566.
185.8333    283.
185.9166      0.
186.5416    283.
```

Branch Inflow Temperature File

This file contains the inflow temperatures for a branch with an upstream flow boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch with an upstream flow boundary condition (see page C8). This allows the user to update temperatures for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The second field is the inflow temperature, °C.

Example

```
CE-QUAL-W2 sample inflow temperature file

     JDAY      TIN
     1.00     6.80
     2.00     6.70
     3.00     7.00
     4.00     6.30
     5.00     6.40
     6.00     6.10
     7.00     6.60
     8.00     5.70
     9.00     5.20
    10.00     5.40
    11.00     7.10
    12.00     6.60
    13.00     5.50
    14.00     5.60
    15.00     7.30
    16.00     9.50
```

Branch Inflow Constituent Concentration File

This file contains the inflow concentrations for a branch with an upstream flow boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. *If* constituents are being modeled, a separate file is required for each branch with an upstream flow boundary condition (see page C8). This allows the user to update constituent concentrations for one branch independent of another branch.
2. Input format for all fields is F8.0 which allows the user to specify the decimal point location. The number of fields is determined by (6) below and are always located on one line.
3. The first two lines are ignored and can be used to comment the file.
4. The next line contains the abbreviations for the constituent names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The remaining fields contain the concentration for each constituent specified on the **Inflow Active Constituent Control** card (see page C75). Only those constituents specified as *active* on the Inflow Active Constituent control card are included in the constituent inflow concentration file. In the following example, only coliform bacteria has been included in level **I** while level **III** has been left out entirely.

Example

CE-QUAL-W2 constituent inflow concentration sample input file

JDAY	CLFORM	SSOLID	L DOM	R DOM	ALGAE	DETRIT	PO4	NH4	NO3	O2	Fe
1.	17.	62.	7.333	17.111	0.0	0.9	0.02	0.10	0.42	13.9	0.4
8.	13.	0.	8.000	18.667	0.0	0.4	0.01	0.03	0.37	14.0	0.2
15.	11.	17.	9.333	21.778	0.0	0.0	0.00	0.01	0.17	10.0	0.3
22.	14.	34.	10.000	23.333	0.0	0.0	0.05	0.00	0.20	10.4	1.6
29.	17.	38.	4.467	10.422	0.0	0.4	0.01	0.11	0.26	11.6	0.4
36.	101.	24.	3.867	9.022	0.0	0.2	0.01	0.00	0.23	12.2	0.3
43.	10.	11.	4.133	9.644	0.0	0.2	0.02	0.07	0.20	12.2	0.1

Branch Outflow File

This file contains the outflow for a branch with a downstream flow boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch with a downstream flow boundary condition. This allows the user to update outflows for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location. There are a maximum of 10 fields to a line. If there are *more* outflows than can be specified on one line, then they are continued on the next line with blanks inserted in the Julian date field.
3. The first two lines are ignored and can be used to comment the file.
4. The next line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The remaining fields are the outflow rate, $m^3 sec^{-1}$.
7. If the selective withdrawal option is used, then a separate column of outflow values must be specified for each outlet structure (see page C24)
8. If the selective withdrawal option is not used, then outflows from a single outlet structure spanning more than one layer in the computational grid can be divided up into several outflows and the total outflow apportioned among them.

Example

CE-QUAL-W2 sample outflow file

JDAY	QOUT	QOUT	QOUT	QOUT	QOUT	QOUT	QOUT	QOUT	QOUT
1.00	8.13	8.13	8.13						
2.00	6.77	6.77	6.77						
3.00	18.60	18.60	18.60						
4.00	0.60	0.60	0.60						
5.00	7.50	7.50	7.50						
6.00	2.87	2.87	2.87						

Withdrawal File

This contains the outflow for each withdrawal specified on the **Number of Withdrawals** card (see page C32). The following is a list of guidelines for file preparation:

1. The order in which withdrawal outflows appear in the file *must* correspond with the order specified on the Withdrawal Segment and the **Withdrawal Layer** cards (see pages C33-C34).
2. Input format for each field is F8.0 with 10 fields to a line. The F8.0 input field allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The remaining fields are the withdrawal outflow rate, $m^3 \, sec^{-1}$
7. Outflows from a single withdrawal structure spanning more than one layer in the computational grid can be divided up into several outflows and the total outflow apportioned among them.
8. If there are *more* withdrawals than can be specified on one line, then they are continued on the next line with blanks inserted under the JDAY field.

Example

CE-QUAL-W2 sample withdrawal outflow file

JDAY	QWD	QWD	QWD	QWD	QWD	QWD	QWD	QWD	QWD
182.0000	51. 51.	51.	51.	51.	51.	51.	51.	51.	51.
182.2500	0. 0.	0.	0.	0.	0.	0.	0.	0.	0.
183.0000	51. 51.	51.	51.	51.	51.	51.	51.	51.	0.
183.2500	0. 0.	0.	0.	0.	0.	0.	0.	0.	0.

Tributary Inflow File

This file contains the inflows for a tributary specified on the **Tributary Segment** card (see page C37). The following is a list of guidelines for file preparation:

1. A separate file is required for each tributary. This allows the user to update inflows for one tributary independent of another tributary.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The second field is the inflow rate, $m^3 \, sec^{-1}$.

Example

```
CE-QUAL-W2 sample tributary inflow file

   JDAY    QTRIB
    1.0     22.8
    5.0     44.5
   12.0     31.2
   23.0     80.4
   35.0     50.6
   74.5    103.0
   74.7    185.6
   75.0    212.3
   75.5    178.6
   80.0    123.4
   80.5     78.3
   90.0     46.5
  112.0     35.9
```

Tributary Inflow Temperature File

This file contains the inflow temperatures for a tributary specified on the **Tributary Segment** card (see page C37). The following is a list of guidelines for file preparation:

1. A separate file is required for each tributary. This allows the user to update inflow temperatures for one tributary independent of another tributary.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The second field is the inflow temperature, $°C$.

Example

```
CE-QUAL-W2 sample tributary inflow temperature file

    JDAY    TTRIB
     1.0     10.3
     5.0      9.5
    12.0     10.1
    23.0      8.6
    35.0     11.2
    74.5     13.9
    74.7     13.1
    75.0     12.8
    75.5     12.5
    80.0     12.6
    80.5     12.7
    90.0     15.4
```

Tributary Inflow Concentration File

This file contains the inflow constituent concentrations for each tributary specified on the **Tributary Segment** card (see page C37). The following is a list of guidelines for file preparation:

1. *If* constituents are being modeled, a separate file is required for each tributary. This allows the user to update constituent inflow concentrations for one tributary independent of another tributary.
2. Input format for all fields is F8.0 which allows the user to specify the decimal point location. The number of fields is determined by (6) below and are always located on one line.
3. The first two lines are ignored and can be used to comment the file.
4. The next line contains the abbreviations for the constituent names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The remaining fields contain the concentration for each constituent specified on the **Tributary Active Constituent Control** card (see page C76). Only those constituents specified as *active* on the control card may be included in the tributary inflow concentration file. In the following example, only coliform bacteria has been included in level **I** while level **III** has been left out entirely.

Example

```
    CE-QUAL-W2 sample tributary constituent inflow concentration file

JDAY CLFORM SSOLID  L DOM  R DOM  ALGAE DETRIT    PO4    NH4    NO3     O2    Fe
  1.    17.    62.  7.333 17.111   0.0    0.9    0.02   0.10   0.42   13.9   0.4
  8.    13.    0.0  8.000 18.667   0.0    0.4    0.01   0.03   0.37   14.0   0.2
 15.    11.    17.  9.333 21.778   0.0    0.0    0.00   0.01   0.17   10.0   0.3
 22.    14.    34. 10.000 23.333   0.0    0.0    0.05   0.00   0.20   10.4   1.6
 29.    17.    38.  4.467 10.422   0.0    0.4    0.01   0.11   0.26   11.6   0.4
 36.   101.    24.  3.867  9.022   0.0    0.2    0.01   0.00   0.23   12.2   0.3
 43.    10.    11.  4.133  9.644   0.0    0.2    0.02   0.07   0.20   12.2   0.1
```

Branch Distributed Tributary Inflow File

This file contains the inflows for a distributed tributary specified on the **Distributed Tributaries** card (see page C40). The following is a list of guidelines for file preparation:

1. A separate file is required for each distributed tributary. This approach allows the user to update inflows for one distributed tributary independent of another distributed tributary.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The second field is the inflow rate, $m^3 \, sec^{-1}$.

Example

```
CE-QUAL-W2 sample distributed tributary inflow file

 JDAY   QDTRIB
  1.0     22.8
  5.0     44.5
 12.0     31.2
 23.0     80.4
 35.0     50.6
 74.5    103.0
 74.7    185.6
 75.0    212.3
 75.5    178.6
 80.0    123.4
 80.5     78.3
 90.0     46.5
```

Branch Distributed Tributary Inflow Temperature File

This file contains the inflow temperatures for a distributed tributary specified on the **Distributed Tributary** card (see page C40). The following is a list of guidelines for file preparation:

1. A separate file is required for each distributed tributary. This allows the user to update inflow temperatures for one distributed tributary independent of another distributed tributary.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The second field is the inflow temperature, $°C$.

Example

```
CE-QUAL-W2 sample tributary inflow temperature file

   JDAY   TDTRIB
    1.0    10.3
    5.0     9.5
   12.0    10.1
   23.0     8.6
   35.0    11.2
   74.5    13.9
   74.7    13.1
   75.0    12.8
   75.5    12.5
   80.0    12.6
   80.5    12.7
```

Branch Distributed Tributary Inflow Concentration File

This file contains the distributed tributary constituent concentrations for each branch (see page C40). The following is a list of guidelines for file preparation:

1. *If* constituents are being modeled, a separate file is required for each branch. This allows the user to update constituent inflow concentrations for one branch independent of another branch.
2. Input format for all fields is F8.0 which allows the user to specify the decimal point location. The number of fields is determined by (6) below and are always located on one line.
3. The first two lines are ignored and can be used to comment the file.
4. The next line contains the abbreviations for the constituent names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The remaining fields contain the concentration for each constituent specified on the **Distributed Tributary Active Constituent Control** card (see page C77). Only those constituents specified as *active* on the control card may be included in the distributed tributary inflow concentration file. In the following example, only coliform bacteria has been included in level I while level III has been left out entirely.

Example

```
CE-QUAL-W2 sample distributed tributary constituent inflow concentration file

JDAY CLFORM SSOLID  L DOM  R DOM  ALGAE DETRIT   PO4    NH4    NO3    O2    Fe
  1.    17.    62.  7.333 17.111   0.0    0.9   0.02   0.10   0.42  13.9   0.4
  8.    13.    0.0  8.000 18.667   0.0    0.4   0.01   0.03   0.37  14.0   0.2
 15.    11.    17.  9.333 21.778   0.0    0.0   0.00   0.01   0.17  10.0   0.3
 22.    14.    34. 10.000 23.333   0.0    0.0   0.05   0.00   0.20  10.4   1.6
 29.    17.    38.  4.467 10.422   0.0    0.4   0.01   0.11   0.26  11.6   0.4
```

Branch Precipitation File

This file contains the precipitation values for a branch and is needed only if the precipitation option [PRCPC] is turned on (see page C12). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch. This allows the user to update precipitation for one branch independent of another branch if needed.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The second field is the precipitation rate, $m\ sec^{-1}$.

Note the following example takes advantage of the algorithm's capability to use data at varying frequencies.

Example

```
CE-QUAL-W2 sample precipitation file

    JDAY   PRECP
182.0000   0.000
182.5416   0.001
182.6250   0.002
182.6666   0.000
188.475    0.002
189.500    0.000
```

Branch Precipitation Temperature File

This file contains the precipitation temperatures for a branch and is needed only if the precipitation option [PRCPC] is turned on (see page C12). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch. This allows the user to update temperatures for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The second field is the precipitation temperature, $°C$.

Example

```
CE-QUAL-W2 sample precipitation temperature file

    JDAY      TPR
    1.00      6.80
    2.00      6.70
    3.00      7.00
    4.00      6.30
    5.00      6.40
    6.00      6.10
    7.00      6.60
    8.00      5.70
    9.00      5.20
   10.00      5.40
   11.00      7.10
   12.00      6.60
```

Branch Precipitation Concentration File

This file contains the precipitation concentrations for a branch and is needed only if the precipitation option [PRCPC] is turned on (see page C12). The following is a list of guidelines for file preparation:

1. *If* constituents are being modeled, a separate file is required for each branch. This allows the user to update constituent concentrations for one branch independent of another branch.
2. Input format for all fields is F8.0 which allows the user to specify the decimal point location. The number of fields is determined by (6) below and are always located on one line.
3. The first two lines are ignored and can be used to comment the file.
4. The next line contains the abbreviations for the constituent names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The remaining fields contain the concentration for each constituent specified on the **Precipitation Active Constituent Control** card (see page C78). Only those constituents specified as *active* on the Precipitation Active Constituent control card may be included in the constituent inflow concentration file. In the following example, only DO has been included.

Example

```
CE-QUAL-W2 constituent precipitation concentration sample input file

     JDAY        DO
  180.000       8.7
  190.000       8.2
  195.000       8.0
  220.000       7.8
```

Branch External Upstream Head Elevation File

This file contains the elevations for a branch with an external upstream head boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch with an external upstream head boundary condition. This allows the user to update elevations for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The next line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The next field is the external head elevation (m above datum specified on the **Initial Condition** card, page C11).

Example

```
CE-QUAL-W2 sample external head elevation file

    JDAY    ELUH
 180.000  431.12
 180.050  431.15
 180.100  431.20
 180.150  431.25
 180.200  431.30
```

Branch External Upstream Head Temperature File

This file contains the upstream temperature profiles for a branch with an external upstream head boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch. This allows the user to update temperatures for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The next fields are the upstream boundary temperatures, $^\circ C$
7. Temperature values must be specified for each cell starting from layer two and extending to the bottom active layer at the upstream segment. If the values do not all fit on one line, then they are continued on the next line with the first field (corresponding to the Julian date field) left blank. The reason why the temperatures must start at layer two is the water surface may vary over many layers during the simulation and it is impossible to know beforehand exactly what time layers will be added or subtracted. When preparing the boundary temperature profiles, it is best to assign boundary temperatures starting from the bottom layer. Once the surface layer has been reached, then use this value to assign values up to layer two. In the following example, the surface layer [KT] starts out at layer six and and the bottom is at layer 22. The first four values correspond to layers two through five and must be defined even if they are never used.

Example

```
            CE-QUAL-W2 sample external upstream boundary temperature file
     JDAY    TUH     TUH     TUH     TUH     TUH     TUH     TUH     TUH     TUH
  180.500    19.3    19.3    19.3    19.3    19.3    19.0    18.8    18.7    18.6
             18.4    18.0    17.0    15.0    14.0    13.5    13.2    13.0    12.8
             12.8    12.8    12.8
  187.500    20.3    20.3    20.3    20.3    20.3    20.0    19.8    19.7    19.6
             19.4    19.0    18.0    15.5    14.0    13.5    13.2    13.0    12.8
             12.8    12.8    12.8
```

Branch External Upstream Head Constituent Concentration File

This file contains the upstream constituent concentration profiles for a branch with an external upstream head boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. *If* constituents are being modeled, then a separate file is required for each branch. This allows the user to update temperatures for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The next fields are the upstream boundary constituent concentrations.
7. Constituents must appear in the same order as they are turned on in the **Active Constituent** card (see page C71). A boundary concentration is *required for each* active constituent.
8. Concentration values must be specified for each cell starting from layer two and extending to the bottom active layer at the upstream segment. If the values do not all fit on one line, then they are continued on the next line with the first field (corresponding to the Julian date field) left blank. The reason why the concentrations must start at layer two is the water surface may vary over many layers during the simulation and it is impossible to know beforehand exactly what time layers will be added or subtracted. When preparing the boundary concentration profiles, it is best to assign concentrations starting from the bottom layer. Once the surface layer has been reached, then use this value to assign values up to layer two. In the following example, the surface layer [KT] starts out at layer six and and the bottom is at layer 22. The first four values correspond to layers two through five and must be defined even if they are never used. Salinity and dissolved oxygen are the only values specified as active.

Example

```
CE-QUAL-W2 sample external upstream boundary constituent concentration file
    JDAY     CUH     CUH     CUH     CUH     CUH     CUH     CUH     CUH     CUH
 180.000    23.5    23.5    23.5    23.5    23.5    23.9    24.5    25.0    26.0
            27.0    28.0    29.0    29.5    30.0    30.2    30.4    30.6    30.6
            30.6    30.6    30.6    30.6
 180.000     9.0     9.0     9.0     9.0     9.0     9.0     9.0     8.8     8.7
             8.6     8.4     8.0     7.5     7.0     6.0     5.5     5.5     5.5
             5.5     5.5     5.5     5.5
 190.000    23.5    23.5    23.5    23.5    23.5    23.9    24.5    25.0    26.0
            27.0    28.0    29.0    29.5    30.0    30.2    30.4    30.6    30.6
            30.6    30.6    30.6    30.6
 190.000     9.0     9.0     9.0     9.0     9.0     9.0     9.0     8.8     8.7
             8.6     8.4     8.0     7.0     6.0     5.0     5.0     5.0     5.0
             5.0     5.0     5.0     5.0
```

Branch External Downstream Head Elevation File

This file contains the elevations for a branch with an external downstream head boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch with an external downstream head boundary condition. This allows the user to update elevations for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The next line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The next field is the external head elevation (m above datum specified on the **Initial Condition** card, page C11).

Example

```
CE-QUAL-W2 sample external downstream head elevation file

    JDAY    ELUH
 180.000  431.12
 180.050  431.15
 180.100  431.20
 180.150  431.25
 180.200  431.30
```

Branch External Downstream Head Temperature File

This file contains the downstream temperature profiles for a branch with an external downstream head boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch. This allows the user to update temperatures for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The next fields are the downstream boundary temperatures, °C
7. Temperature values must be specified for each cell starting from layer two and extending to the bottom active layer at the downstream segment. If the values do not all fit on one line, then they are continued on the next line with the first field (corresponding to the Julian date field) left blank. The reason why the temperatures must start at layer two is the water surface may vary over many layers during the simulation and it is impossible to know beforehand exactly what time layers will be added or subtracted. When preparing the boundary temperature profiles, it is best to assign boundary temperatures starting from the bottom layer. Once the surface layer has been reached, then use this value to assign values up to layer two. In the following example, the surface layer [KT] starts out at layer six and and the bottom is at layer 22. The first four values correspond to layers two through five and must be defined even if they are never used.

Example

CE-QUAL-W2 sample external downstream boundary temperature file

JDAY	TUH	TUH	TUH	TUH	TUH	TUH	TUH	TUH	TUH
180.500	19.3	19.3	19.3	19.3	19.3	19.0	18.8	18.7	18.6
	18.4	18.0	17.0	15.0	14.0	13.5	13.2	13.0	12.8
	12.8	12.8	12.8						
187.500	20.3	20.3	20.3	20.3	20.3	20.0	19.8	19.7	19.6
	19.4	19.0	18.0	15.5	14.0	13.5	13.2	13.0	12.8
	12.8	12.8	12.8						

Branch External Downstream Head Concentration File

This file contains the downstream constituent concentration profiles for a branch with an external downstream head boundary condition (see page C8). The following is a list of guidelines for file preparation:

1. A separate file is required for each branch. This allows the user to update temperatures for one branch independent of another branch.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains the variable names which are right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is the Julian date which can be entered at any frequency. The frequency between updates may vary during the simulation.
6. The next fields are the downstream boundary constituent concentrations.
7. Constituents must appear in the same order as they are turned on in the **Active Constituent** card (see page C71). A boundary concentration profile is *required for each* active constituent.
8. Concentration values must be specified for each cell starting from layer two and extending to the bottom active layer at the downstream segment. If the values do not all fit on one line, then they are continued on the next line with the first field (corresponding to the Julian date field) left blank. The reason why the concentrations must start at layer two is the water surface may vary over many layers during the simulation and it is impossible to know beforehand exactly what time layers will be added or subtracted. When preparing the boundary concentration profiles, it is best to assign concentrations starting from the bottom layer. Once the surface layer has been reached, then use this value to assign values up to layer two. In the following example, the surface layer [KT] starts out at layer six and and the bottom is at layer 22. The first four values correspond to layers two through five and must be defined even if they are never used. Salinity and dissolved oxygen are the only values specified as active.

Example

CE-QUAL-W2 sample external downstream boundary constituent concentration file

JDAY	CUH	CUH	CUH	CUH	CUH	CUH	CUH	CUH	CUH
180.000	23.5	23.5	23.5	23.5	23.5	23.9	24.5	25.0	26.0
	27.0	28.0	29.0	29.5	30.0	30.2	30.4	30.6	30.6
	30.6	30.6	30.6	30.6					
180.000	9.0	9.0	9.0	9.0	9.0	9.0	9.0	8.8	8.7
	8.6	8.4	8.0	7.5	7.0	6.0	5.5	5.5	5.5
	5.5	5.5	5.5	5.5					
190.000	23.5	23.5	23.5	23.5	23.5	23.9	24.5	25.0	26.0
	27.0	28.0	29.0	29.5	30.0	30.2	30.4	30.6	30.6
	30.6	30.6	30.6	30.6					
190.000	9.0	9.0	9.0	9.0	9.0	9.0	9.0	8.8	8.7
	8.6	8.4	8.0	7.0	6.0	5.0	5.0	5.0	5.0
	5.0	5.0	5.0	5.0					

Vertical Profile File

This file contains a single vertical profile used to specify initial conditions for temperatures and/or constituent concentrations. The vertically varying profile is then used to initialize all segments in the computational grid. This file is most commonly used for vertically stratified waterbodies with no longitudinal gradients. The following is a list of guidelines for file preparation:

1. An initial vertical profile is specified by inputting -1.0 for the initial temperature on the **Initial Conditions** card or a constituent's initial concentration on the **Initial Concentration** card (see pages C11 and C73). If temperature is included, then it *must* be the first profile in the file. Constituent profiles *must* be input in the same order as they are specified on the **Initial Concentration** card.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains in the first field a constituent identifier name to aid in creating and editing the file. The remaining fields contain the variable name which is right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is left blank or can be used for comments since it is ignored on input. The remaining fields are used for specifying the temperature or concentration at a given layer. If there are *more* values than can be specified on one line, then they are continued on the next line leaving the first field blank or using it for comments.
6. Values for the vertical profile start at the water surface layer [KT] and stop at the bottom layer. Boundary segments are *not* included in the file.

The following sample input file contains vertically varying initial temperature and dissolved oxygen profiles which correspond to the sample input bathymetry. The surface layer [KT] is located at layer five.

Example

CE-QUAL-W2 sample vertical profile initial conditions file

```
TEMP VPR     T1     T1     T1     T1     T1     T1     T1     T1     T1
            15.2   15.0   14.7   14.5   14.3   14.2   11.7    8.5    6.7
             6.2    6.0    6.0    6.0    6.0    6.0    6.0    6.0    6.0
             6.0    6.0

DO VPR       C1     C1     C1     C1     C1     C1     C1     C1     C1
            12.0   12.0   12.0   12.0   11.9   11.9   11.7    8.5    6.7
             6.2    6.0    6.0    6.0    6.0    6.0    6.0    6.0    6.0
             6.0    6.0
```

Longitudinal Profile File

This file contains vertical profiles for each segment used to initialize temperature and/or constituent concentrations for each computational grid cell. It is useful when temperature or a constituent is both vertically and longitudinally stratified where a single value or profile is not representative of the initial conditions. The following is a list of guidelines for file preparation:

1. An initial longitudinal profile input is specified by inputting -2.0 for the initial temperature on the **Initial Conditions** card or a constituent's initial concentration on the **Initial Concentration** card (see pages C11 and C73). If temperature is included, then it *must* be the first series of profiles in the file. Constituent profiles *must* be input in the same order as they are specified on the **Initial Concentration** card.
2. Input format for each field is F8.0 which allows the user to specify the decimal point location.
3. The first two lines are ignored and can be used to comment the file.
4. The third line contains in the first field a constituent identifier name to aid in creating and editing the file. The remaining fields contain the variable name which is right justified according to the input field. This line is also ignored although the preprocessor checks to ensure the fields are aligned correctly.
5. The first field is left blank or can be used for comments since it is ignored on input. The remaining fields are used for specifying the temperature or concentration at a given layer. If there are *more* values than can be specified on one line, then they are continued on the next line leaving the first field blank or using it for comments.
6. Values for the vertical profile at each segment start at the water surface layer [KT] and stop at the bottom layer. Boundary segments are *not* included in the file.

The following sample input file includes vertically and longitudinally varying initial conditions for temperature and dissolved oxygen which corresponds to the sample input bathymetry. The surface layer [KT] is located at layer 5.

Example

```
                    CE-QUAL-W2 sample longitudinal profile file
Segment 2
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.0    14.8    14.5    14.3    14.2    14.1    11.5    8.2     6.5
             6.2     6.0     6.0
Segment 3
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.0    14.8    14.5    14.3    14.2    14.1    11.5    8.2     6.5
             6.2     6.0
Segment 4
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.0    14.8    14.5    14.3    14.2    14.1    11.5    8.2     6.5
             6.2
Segment 5
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.0    14.8    14.5    14.3    14.2    14.1    11.5    8.2     6.5
Segment 6
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.1    14.9    14.5    14.4    14.2    14.2    11.7    8.5     6.7
             6.2     6.0     6.0
Segment 7
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.1    14.9    14.6    14.4    14.2    14.2    11.7    8.5     6.7
             6.2     6.0     6.0     6.0     6.0     6.0
Segment 8
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.2    15.0    14.7    14.5    14.3    14.2    11.7    8.5     6.7
             6.2     6.0     6.0     6.0     6.0     6.0     6.0     6.0     6.0
Segment 9
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.2    15.0    14.7    14.5    14.3    14.2    11.7    8.5     6.7
             6.2     6.0     6.0     6.0     6.0     6.0     6.0     6.0     6.0
             6.0     6.0
Segment 12
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.5    15.3    14.8    14.5    14.3    14.2    10.6    7.2
Segment 13
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.4    15.2    14.8    14.5    14.3    14.2    10.6    7.2     6.8
             6.2     6.0
Segment 14
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.4    15.2    14.8    14.5    14.3    14.2    10.6    7.2     6.5
             6.2     6.0     6.0     6.0
Segment 15
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.5    15.3    14.8    14.5    14.3    14.2    10.6    7.2     6.4
             6.2     6.0     6.0     6.0     6.0
Segment 18
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.5    15.3    14.8    14.5    14.3    14.2    10.6    7.2     6.4
             6.2     6.0     6.0     6.0     6.0     6.0     6.0     6.0
Segment 19
Temperature  T1      T1      T1      T1      T1      T1      T1      T1      T1
             15.5    15.3    14.8    14.5    14.3    14.2    10.6    7.2     6.4
             6.2     6.0     6.0     6.0     6.0     6.0     6.0     6.0     6.0
             6.0
```

```
Segment 2
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.5    8.2     6.5
         6.2     6.0     6.0
Segment 3
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.5    8.2     6.5
         6.2     6.0
Segment 4
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.5    8.2     6.5
         6.2
Segment 5
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.5    8.3     6.5
         6.2     6.0
Segment 6
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.6    8.4     6.7
         6.2     6.0     6.0
Segment 7
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.6    8.5     6.7
         6.2     6.0     6.0     6.0     6.0     6.0
Segment 8
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.6    8.5     6.7
         6.2     6.0     6.0     6.0     6.0     6.0     6.0     6.0     6.0
Segment 9
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.7    8.5     6.7
         6.2     6.0     6.0     6.0     6.0     6.0     6.0     6.0     6.0
         6.0     6.0
Segment 12
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    15.3    14.8    14.5    14.3    14.2    11.7    8.5
Segment 13
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.7    8.5     6.8
         6.2     6.0
Segment 14
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.7    8.5     6.5
         6.2     6.0     6.0     6.0
Segment 15
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.7    8.5     6.4
         6.2     6.0     6.0     6.0     6.0
Segment 18
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.7    8.5     6.4
         6.2     6.0     6.0     6.0     6.0     6.0     6.0     6.0
Segment 19
DO       C1      C1      C1      C1      C1      C1      C1      C1      C1
         12.0    12.0    12.0    12.0    11.9    11.9    11.7    8.5     6.4
         6.2     6.0     6.0     6.0     6.0     6.0     6.0     6.0     6.0
         6.0
```

Appendix D
Description of Algorithms

Introduction

Programming Philosophy. The basic philosophy behind the coding of CE-QUAL-W2 is that the present code is not the end of the model's development. Any good code recognizes this and facilitates future improvements. Code should not be static and should accommodate, with minimal effort, advances in the state-of-the-art in hydrodynamics, numerical solutions, water quality interactions, and computer software and hardware.

Unfortunately, most water quality models were written for mainframe computers oriented towards card deck inputs by people with little formal training in computer programming. Many models were written by engineers whose goal during code development was to have the code give correct answers on their computers for the problem being addressed. Little thought was given to the fact that if the program was to be useful, then it should be applicable to different problems and by other people using different computers. The code that can be applied to only one problem by only one person on only one type of computer should probably have never been written in the first place.

Many water quality modelers also ardently believe the only people who should apply water quality models should be experts. This philosophy has its merit. Many criticisms aimed at water quality modeling (much of it deserved) are due to the misapplication of a model by a person only vaguely familiar with water quality modeling and even less familiar with the model he heard about through a colleague or at a scientific meeting. To keep the model out of the hands of novices, many code developers knowingly made a model hard to use, or at least resisted improving the model to make it easier to use, so only very determined people would use the model. Unfortunately, a person who is bound and determined to misapply a model will discover a way to do so regardless of the best efforts of the code developer. Putting obstacles up to deter an unqualified user also hinders the qualified user. Even more unfortunately, models are not being used to give cost effective guidance to decision makers because they are too difficult, time consuming, and expensive to use.

One of the major goals in revising the model was to make it easier to understand and thus more maintainable, and easier to use and thus more widely used. The code has been revised according to the following principles:

1. **Easily understandable code.** For a code to evolve, it must be easily understood. People responsible for maintaining codes come and go and it should not involve man-years of effort for a new person to thoroughly understand 6,000 lines of code. FORTRAN is called a language for a good reason. Its primary reason for coming into being was *not* to communicate with the computer. A computer is much happier being given binary instructions. Indeed, this is the only language a computer understands. Rather, FORTRAN was devised to communicate among people - either the person writing the program or someone who comes along after the program is written. CE-QUAL-W2 has been rewritten with this in mind.

   The coding has been extensively reformatted to make the program visually easier to read. A person uses his eyes first in the process of understanding a written language before the thinking portion of the brain is ever engaged. It is easier and faster to discern the logic of a code if the logical structure stands out to the eye. The user should not have to expend more brainpower just to see an algorithm than to understand it. Imagine how much more difficult this manual would be to read and understand if it were not broken down into parts, sections, paragraphs, and sentences - yet a great deal of code is still written this way.

   The code has been rewritten according to top-down programming principles. The code logic structure starts at the program beginning and proceeds downwards. The autostepping algorithm is the only place in the code using a GO TO statement to jump around code. The algorithm could have been coded without the statement, but this is one of the few instances where the code is actually clearer with it.

   The code has been reorganized into logical units that, for the most part, are self-contained. For example, inputs occur only in the input section. The model does not read in a portion of the input data, process it, and then read in more data. If the user needs to modify the input data, he knows exactly where to go in the code.

Unlike many large programs, CE-QUAL-W2 does not have a main program that is essentially a driver for a series of subroutines. The reasoning is the basic model consists of solving the hydrodynamic and then the transport equations. This is what the program does and this is what the user sees when investigating the code. If changes are made to this portion of the code, they can have far reaching effects because the coding in the main program is intimately tied together. The organization reflects this. The model does have subroutines but their coding does not directly affect the main program. For example, changes to the water quality subroutines have no effect on how the main program solves the hydrodynamic and transport equations. Another benefit of this programming approach is the model runs faster when not burdened with the overhead of many subroutine calls.

Logical variables are used extensively throughout the code resulting in self-documenting and easier to understand code. There is a reason why they are called LOGICAL variables. They improve the understanding of the code logic.

It is recognized the code is still incomplete and improvements will be made in the future. In addition, experience has shown almost every application has some unique aspect requiring coding changes. A usable piece of code recognizes these facts and is constructed so changes to the code, although daunting, are not impossible. It is hoped users will make changes to the code to increase the model's utility. However, a word of warning is appropriate. If you make changes, *make certain they are consistent with the programming style in the code*. It is extremely difficult to read reports written by several authors each using a different style of writing. It is almost impossible to understand FORTRAN code pieced together by many different programmers each with their own widely varying style (or in many cases, lack of it).

A few additional comments regarding nomenclature in the code. A large effort was put into making the nomenclature as consistent as possible to make the code understandable. The following list describes conventions for much of the nomenclature in the code. Note these are general guidelines and exceptions do exist.

1. variables beginning with I and K refer to variables associated with segments and layers, respectively - variables beginning with I may also refer to initial conditions
2. variables ending with a 1 or 2 refer to variables occurring at two different time levels

3. variables beginning with S refer to variables whose values are saved - most of these variables are used in the autostepping algorithm
4. variables ending with a T refer to variables whose value changes temporarily and then is reset, or variables that refer to longitudinal or vertical transport
5. variables starting with Q refer to flow associated variables
6. variables ending in C refer to control variables that turn on/off or select various computations to be performed in the code
7. variables beginning with C refer to variables associated with constituents
8. variables ending in BR refer to branch related variables
9. variables beginning with VOL refer to volume related variables
10. variables ending in P refer to pointers to arrays
11. variables ending in PR refer to print related variables

Outline of CE-QUAL-W2

An outline of the code listing the major algorithms is given below. Parts of this outline are direct implementations of the hydrodynamic and transport computations (Tasks 2.2 and 2.3) and their accompanying initial and boundary conditions (Task 1.4.4 and Task 2.2.1) presented in Appendix A. The remaining tasks are related to algorithms described in this Appendix.

Task 1: Initialization
 Task 1.1: Common Block
 Task 1.2: Program
 Task 1.3: Inputs
 Task 1.4: Variables
  Task 1.4.1: Zero Variables
  Task 1.4.2: Miscellaneous Variables
  Task 1.4.3: Geometry
  Task 1.4.4: Initial Conditions
 Task 1.5: Outputs
Task 2: Calculations
 Task 2.1: Hydrodynamic Sources/Sinks
 Task 2.2: Hydrodynamic Calculations
  Task 2.2.1: Boundary Concentrations, Temperatures, and Densities
  Task 2.2.2: Momentum Terms
  Task 2.2.3: Water Surface Elevation
  Task 2.2.4: Longitudinal Velocities
  Task 2.2.5: Vertical Velocities
  Task 2.2.6: Autostepping

Task 2.3: Temporal Balance Terms and Temperatures
Task 2.4: Constituents
Task 2.5: Layer - Segment Addition and Subtraction
Task 2.6: Balances
Task 2.7: Update Variables for Next Timestep
Task 2.8: Output Results
Task 3: End Simulation

The reader should refer to the code and Appendix C, Input Data Description, while studying the following description of the model code.

Task 1: Initialization

All of the code dealing with setting up the model for a simulation is located in this task. This includes variable declarations and initializations, initial conditions input and grid setup, and output initialization.

Task 1.1: Common Block

This section of code contains the data statements for variables in named common areas. ANSI standard Fortran restricts data initialization of common blocks to block data subprograms.

Task 1.2: Program

Type declarations
Dimension statements
Common declarations
Data statements

The separate include file, W2.INC, contains the PARAMETER, DIMENSION, and EQUIVALENCE statements, and type declarations global to the code. It also establishes a common area for the constituent concentrations and their sources/sinks. The PARAMETER statements in the include file specify the name of the control file and the array dimensions that depend on the grid size used to represent the waterbody being modeled.

The equivalence statements allow the kinetics subroutines to be written using easily understandable variable names (e.g., [ALGAE] instead of [C2]) while still allowing simple DO loops in the main code.

Following the include statement are type declarations, dimension statements and specification of common areas. An attempt has been made to logically group the variables according to their usage in the code.

Task 1.3: Inputs

Open control file
　　Read title cards
　　Read time control cards
　　Read grid definition cards
　　Read initial condition cards
　　Read inflow-outflow cards
　　Read output control cards (excluding constituents)
　　Read constituent control cards
　　Read kinetics coefficients
　　Read input filenames
　　Read output filenames
Read bathymetry file
Initialize logical control variables
Initialize temperature and constituents
Read restart data
Close files
Input FORMATs

This code section reads data from the control file [CONFN], the bathymetry file [BTHFN], the vertical profile file [VPRFN] and/or the longitudinal-vertical profile file [LPRFN], and the restart file [RSIFN]. These files contain all of the inputs necessary for a simulation except for time-varying boundary condition data used during the simulation. In general, the control file sets up initial conditions for the simulation. The inputs are broken into sections that are as similar as possible.

The bathymetry file contains geometric information to initialize the computational grid. The information includes the segment lengths [DLX], the layer heights [H], the water surface elevation for each segment [Z1], the orientation for each segment [PHI0], and the average widths for each cell in the grid [B].

A preliminary section of logical variables are initialized in this section because of their necessity when the code evaluates whether or not to read initial conditions for temperature and/or constituents from a file containing a single vertical profile [VPRFN] and/or a file containing a vertical profile *for each segment* [LPRFN]. The next piece of code runs through the logic necessary for deter-

mining if either of these two files are used to set initial conditions and proceeds as follows:

The variables [IT2] and [IC2] which were input in the control file are used to determine if initial temperatures and/or concentrations will be obtained from information in these files. If either [IT2] for temperature or [IC2] for any constituent is set to -1, then the logical variable [VERT_TEMP] and/or [VERT_CONC] is set to true and the code then knows information is to be read from the vertical profile file. This file specifies a single vertically varying profile used to initialize temperature and/or constituent concentrations for each segment. If either [IT2] or [IC2] is set to -2, then the logical variable [LONG_TEMP] and/or [LONG_CONC] is set to true and the code then knows information is to be read from the longitudinal-vertical profile file. This file specifies a vertically varying profile *for each segment* used to initialize the grid. The logical variable [OPEN_VPR] is set to true if either [VERT_TEMP] or any of the [VERT_CONC] variables are true. This variable is used in the next section to open the vertical profile file [VPRFN] where the single vertical profile is read into either the array [TVP] and/or [CVP].

Similar logic is used with the [OPEN_LPR] variable except the information is not read in until the initialization section. There are two reasons for doing this. If the information is read in at this point, then the user would have to specify a vertical profile for every segment in the grid starting at segment two. By waiting until the grid geometry is defined, the user need only specify vertical profiles starting at the upstream active segment [IUC]. The second reason is to eliminate the need for a temporary storage array dimensioned (KMP,IMP,NCP) thus reducing memory requirements.

The restart capability of the code permits previous simulations to be continued. The code reads an unformatted file output by a previous run containing all the necessary variables to reproduce exactly the internal state of the code at the end of the previous run. The logical variable RESTART_IN is used to control how the code is initialized for restarts. The reader may trace the use of this variable in the code beginning with the variable [RSIC] which specifies whether input is read in from the restart file (see page C110).

Internally, the file names and corresponding FORTRAN unit numbers are consistently named with the unit numbers corresponding to the input filenames (ie., BTH for unit number, BTHFN for the filename). Unit numbers 10-19 are reserved for input files.

Task 1.4: Variables

This section initializes variables based on the information available from reading the control, bathymetry, vertical profile, and restart files.

Task 1.4.1: Zero Variables

Task 1.4.1 initializes to zero variables used in the code before they are initialized (ie., appear on the right hand side of an assignment statement before being assigned a value). These include source and sink arrays, vertical and horizontal velocities and volume balance variables. Note the logical variable used for restarting the computation [RESTART_IN] to prevent values read in from the restart file from being overwritten:

```
IF (.NOT.RESTART_IN) THEN
  Z1(I) = 0.0
  DO K=1,KMP
    U(K,I) = 0.0
    W(K,I) = 0.0
  END DO
END IF
```

The character array [CONV] is initialized to a series of blanks. This array is used to print water surface elevations, ice cover, velocities, temperatures, vertical eddy viscosities, constituent concentrations and limiting factors for the growth of algae. It permits computed values for these variables to be printed for active cells and blanks to be printed for inactive cells thus improving the readability of the snapshot output.

Task 1.4.2: Miscellaneous Variables

Logical controls
Convert rates from per-day to per-second
Time and printout control variables
Active constituents

This code section converts logic control variables specified in the control file to LOGICAL variables. LOGICAL variables are used extensively throughout the code to make the code more readable. For the most part, the logic associated with setting these variables is inconsequential to understanding what is going on in the code. The user may examine these statements to determine the relationship of the control file inputs (see Appendix C) to the LOGICAL variables.

The logic for identifying winter is used to prevent ice formation after Julian day 40 and before Julian day 300. The logical array [TRANSPORT] is used to

prevent the transport of certain constituents that are not state variables but are secondarily calculated (ie., bicarbonate calculated from alkalinity and total inorganic carbon). Rates are converted from their input values which have units of day^{-1} to the internal units of second^{-1}.

Time variables are initialized next. The variable [JDAY] is used to keep track of the fractional Julian day of the year (ie., 12 noon on January 1 being day 0.5). It is initialized to the starting time [TMSTRT] specified by the user (see page C3). The simulation starting year [YEAR] is an integer value and is read from the control file directly (see page C3). The simulation elapsed time [ELTM] is the time since the start of the simulation, measured in seconds.

A number of other variables depend on these basic time variables. For example, the code allows the user to specify the snapshot output frequency depends on keeping arrays of snapshot dates [SNPD] and frequencies [SNPF] (see pages C47 and C48). This logic requires a pointer [SNPDP] to the current snapshot date and frequency which is initialized in Task 1.4.2. Since the algorithm that locates a particular frequency requires both a beginning and ending date, a final end date must be assigned. This end date is computed as the simulation ending time [TMEND] plus one day:

```
DO J=NSNP+1,NDP
   SNPD(J) = TMEND+1.0
END DO
```

This logic is necessary to prevent the possibility of the snapshot date pointer [SNPDP] pointing to a value past the last specified date in the array. For example, given the following values for the [SNPD] array:

SNP DATE	SNPD	SNPD	SNPD	SNPD	SNPD	SNPD	SNPD	SNPD	SNPD
	100.5	130.5	160.5	190.5	220.5				

If the simulation extended past Julian day 220.5, then the logic for determining when the next snapshot will be output increments [SNPDP] to the next value in the array. Without the preceding initialization, the pointer would be incremented to 6 and the value of [SNPD] would be zero. Since the model's Julian date would be greater than 0.0, a snapshot would be output at every timestep after 220.5. This is eliminated by setting [SNPD(6)] to [TMEND]+1.0. The variables determining when data will be sent to an output file (i.e., [NXTMSN]) are also initialized here. Refer to a description of Task 2.8, page D37 for a more detailed description of the algorithm controlling model output.

The user selects which of the 21 water quality constituents are to be included for a particular application. The next section of code makes a list of the selected constituents:

```
IF (CONSTITUENTS) THEN
  DO JC=1,NCP
    IF (ACC(JC).EQ.' ON') THEN
      NAC      = NAC+1
      CN(NAC) = JC
    END IF
    IF (INACC(JC).EQ.' ON') THEN
      NACIN       = NACIN+1
      INCN(NACIN) = JC
    END IF
    .
    .
    .
    IF (PRACC(JC).EQ.' ON') THEN
      NACPR       = NACPR+1
      PRCN(NACPR) = JC
    END IF
  END DO
END IF
```

The constituent list is [CN]. If the user specified "ON" for a tracer and coliform bacteria on the **Active Constituent Control** card, then [CN] would have the values 1 and 2 only.

This code segment also makes a list of the boundary inputs the user has specified. The boundary inputs consist of inflows, tributaries, distributed tributaries and precipitation. For example, the user may wish to simulate all 21 water quality constituents but may feel comfortable only specifying inflow constituent concentrations for four of them (based on the importance of the boundary inflow or the availability of data). The **Inflow Active Constituent Control** card (see page C75) allows the user to specify which four inflow constituent concentrations will be available. The logic for this procedure is exactly the same as for the active constituents. These arrays are used in the subroutine TIME_VARYING_DATA which is discussed in more detail on page D38.

Task 1.4.3: Geometry

Layer elevations
Bottom layers
Upstream active cell
Boundary bottom layers
Minimum bottom layers
Boundary widths
Areas and bottom widths
Initial water surface and derived geometry
Branch numbers corresponding to tributaries, withdrawals, and head
Branch layer area
Wind fetch lengths
Segment heights

Layer elevations
Beginning and ending segment and bottom layer for snapshots
Transport interpolation multipliers
Positive flows
Negative flows

The variables needed to initialize the waterbody geometry are read in previously in Task 1.3. These variables are the segment length [DLX], the water surface deviation from the top of the initial layer [Z1], the segment orientations [PHI0], and the layer thicknesses [H], all taken from the bathymetry file [BTHFN] (see page C107). Two additional values, the water surface initial layer location [KT] and the elevation at the bottom of the deepest active layer [DATUM] are read from the control file (see page C8).

Task 1.4.3 takes these data and computes variables necessary for the computation. These variables include

1.	layer elevations	[EL]
2.	deepest active cell for each segment	[KB]
3.	upstream active cell for each branch	[CUS]
4.	minimum bottom layer between segment i and $i+1$	[KBMIN]
5.	areas	[BHKT2]
		[BH]
6.	average bottom widths	[BB]
7.	average right-hand side widths	[BR]
8.	branch numbers corresponding to:	
	a. tributaries	[JBTR]
	b. withdrawals	[JBWD]
	c. upstream head	[JBUH]
	d. downstream head	[JBDH]
9.	surface layer thickness	[HKT2]
10.	average layer thickness	[AVHKT2]
		[AVH]
11.	adjusted surface widths	[BKT]
12.	branch layer area	[AKBR]
13.	segment heights	[HSEG]
14.	layer in which the water surface resides	[IKT]

The derived geometry variables are computed once in this section of code and, except for surface related variables which must be updated as the water surface elevation changes, are never recomputed. Most computations are straightforward. However, the algorithm allowing the water surface elevation to extend through multiple layers is described in more detail.

Version 2.0 allows the water surface to extend through multiple layers, whereas in the previous version it was restricted to a maximum of two layers. The variable [IKT] keeps track of which layer the water surface resides in for each segment and is calculated as follows:

```
DO WHILE (EL(KT)-Z1(I).GT.EL(IKT(I)))
   IKT(I) = IKT(I)-1
END DO
```

This section of code takes the elevation [EL] of the user specified surface layer location [KT] and subtracts the deviation from the water surface [Z1]. Remember the deviation upward from the surface layer is defined as negative and the deviation downward is defined as positive, hence [Z1] is subtracted from [EL] to give the actual water surface elevation at a given segment. This value is compared to the layer elevation that [IKT] points to. If the elevation that [IKT] points to is less than the actual water surface elevation, then [IKT] is decremented and the loop is continued until the water surface elevation pointed to by [IKT] is greater than the actual water surface elevation at that segment. After the loop is finished, [IKT] will point to the layer in which the water surface elevation resides. This algorithm requires [EL] be defined beforehand and is the reason why the calculation of [EL] appears first in this section. More details of the variable water surface elevation algorithm are given on page D20.

The bottom active cell [KB] for the internal head boundary segments which attach to branches are assigned the values of [KB] for the segment they attach to. For external heads, [KB] is assigned the value of [KB] at either the upstream or downstream active segment. The same logic is used later in this section to assign the boundary widths [B] for internal head boundary segments.

The assignment of branch numbers where tributaries [JBTRIB], withdrawals [JBWD], and upstream [JBUH] and downstream [JBDH] heads are located is included in this section. Branch layer areas [AKBR], upstream [FETCHU] and downstream [FETCHD] fetch lengths, segment heights [HSEG], and ending [IEPR] segments and bottom layer [KEPR] for printing are also included here. The code is straightforward.

This task is complete with the computation of the transport interpolation multipliers for both positive and negative flow directions. Refer to page A10 for a description of how the multipliers were derived.

Task 1.4.4: Initial Conditions

Temperature
Constituents
Constituent mass
Ice cover
Vertical eddy viscosity
Saved concentrations
Density
Horizontal diffusion
Open output files

This task illustrates some of the typical index sweeps used throughout the remainder of the program. These sweeps are made possible because of variables defined in Task 1.4.3 that identify the current upstream segment for a particular branch [CUS] and the bottom layer number for each segment [KB]. Keep in mind the extent of the sweeps depends on where a particular variable is defined on the computational grid. Variables defined at the center of a cell sweep from the upstream [ID] to the downstream [ID] segments and the surface layer [KT] to the bottom layer [KB]. If the variables are defined at the bottom or right side of a computational cell, then the sweeps are decreased by one.

```
DO JB=1,NBP
  IU = CUS(JB)
  ID = DS(JB)
  IF (.NOT.RESTART_IN) THEN

********* Temperature

    DO I=IU,ID
      IF (LONG_TEMP) READ (LPR,1190) (T1(K,I),K=KT,KB(I))
      DO K=KT,KB(I)
        IF (ISO_TEMP)  T1(K,I) = IT2
        IF (VERT_TEMP) T1(K,I) = TVP(K)
        T2(K,I) = T1(K,I)
      END DO
    END DO
    .
    .
    .
  END IF
  .
  .
  .
******* Horizontal diffusion

    DO I=IU,ID-1
      DO K=KT,KBMIN(I)
        DX(K,I) = IDX
      END DO
    END DO
  END DO
```

The variables ISO_TEMP, VERT_TEMP, and LONG_TEMP are used in the code that initializes the temperature field [T1]. Not only does this section of code demonstrate the use of the logical variables described earlier, but it also shows the use of the segment indices [IU] and [ID]. These indices are stored in arrays by branch number - the current upstream segment [IU] stored in [CUS] and the downstream segment [ID] stored in [DS]. Since temperatures are located at the cell center, their initialization can proceed from the upstream segment [IU] to the downstream segment [ID] and from the top layer [KT] to the bottom layer number for a particular segment [KB].

For horizontal diffusion [DX], which is located at the right-hand side of a cell, use is made of some of the geometric variables computed in Task 1.4.3. The segment loop index [I] extends only to ID-1, since the horizontal diffusion must be maintained at zero along the boundary. The use of the minimum bottom layer number [KBMIN], computed in Task 1.4.3 as KBMIN(I) = MIN(KB(I),KB(I+1)) permits horizontal diffusion to be maintained at zero when the waterbody bottom stairsteps upward.

The saved concentration array [C1S] is initialized here. The array is necessary because the QUICKEST transport algorithm can produce negative values in areas of sharp gradients. The array stores concentrations after they are transported and before negative values are eliminated from the constituent concentrations passed to the kinetic subroutines [C2]. The use of this dual-array system permits perfect mass balances while eliminating negative constituent concentrations from either being displayed or used in the kinetics subroutines.

Task 1.5: Outputs

Open output files
Plot files

This section opens the snapshot [SNPFN], times series [TSRFN], profile [PRFFN], vector plot [VPLFN], and contour plot [CPLFN] files if the user specified output for these files (see pages C46, C57, C52, C60 and C63). The error and warning files (err.opt and wrn.opt) are opened elsewhere when necessary by the code. The restart output file [RSOFN], an unformatted file, is also opened near the end of the main code in the output section. Initial information for the plot file is also written at this time.

Task 2: Calculations

Task 2 integrates the hydrodynamic and transport equations over time. This task is repeated until the simulation is completed. The simulation is initialized at the starting time [TMSTRT] and is completed when the time loop reaches the ending time [TMEND]. The short bit of code under this heading includes the DO WHILE statement that repeats the large number of statements in its range until the ending time is reached. The calls to the subroutines TIME_VARYING_DATA and INTERPOLATE_INPUTS are used to fetch and interpolate time-varying boundary condition data for use in the computations. TIME_VARYING_DATA supplies the boundary data at the correct time. INTERPOLATE_INPUTS linearly interpolates the data which otherwise is supplied to the main code as a step function.

Task 2.1: Hydrodynamic Sources/Sinks

This task incorporates the calculations necessary at the beginning of each time-step before the individual branch calculations are done - distribute outflows using an empirical selective withdrawal algorithm located in the subroutine SELECTIVE_WITHDRAWAL (see page A27), and include various inflows and outflows by assigning them to source and sink arrays. These computations are done for the waterbody as a whole and will be contrasted to similar computations done on a branch-by-branch basis in Task 2.2.1.

The boundary inflows and outflows considered in Task 2.1 are evaporation, precipitation, tributaries, distributed tributaries, withdrawals, and flows to and from other branches.

The following code segment illustrates a typical computation in which a boundary inflow or outflow is added to the hydrodynamic source and sink array [QSS]. This example is the outflow for a user-specified withdrawal. Withdrawals are flows removed from the side of a waterbody, for example, by a generating station's cooling water intake, and are not to be confused with dam releases at a downstream segment.

```
IF (WITHDRAWALS) THEN
  DO JW=1,NWP
    IF (JB.EQ.JBWD(JW)) THEN
      IF (KWD(JW).GE.KT) THEN
        QSS(KWD(JW),IWD(JW)) = QSS(KWD(JW),IWD(JW))-QWD(JW)
      END IF
    END IF
  END DO
END IF
```

The withdrawal rates are supplied by the user through the withdrawal file [QWDFN] (see page C112) and to the model through the subroutine TIME_VARYING_DATA as the array [QWD]. The segment and layer at which the withdrawal occurs are also specified by the user in the control file as the variables [IWD] and [KWD] (see pages C33 and C34). In the code segment, each withdrawal is accessed (JW=1,NWP) by the branch in which it is located. If the withdrawal is at or beneath the current top layer [KT], then the source and sink array is decremented by the withdrawal rate. Note the minus sign for [QWD] representing a sink of water.

This section of code is accessed only if the user has specified at least one withdrawal, which causes the logical variable [WITHDRAWALS] to be set to "true". The branch number for the withdrawal [JBWD] was computed in the initialization section (Task 1.4.3).

Task 2.1 also includes the entry point for restarting the timestep iteration in case the computed timestep [DLT] was too large for the current iteration.

Task 2.2: Hydrodynamic Calculations

The hydrodynamic computations are direct FORTRAN implementations of the finite difference solution described in Appendix A. The reader is encouraged to review this Appendix before studying the code and the following narrative, which concentrates on the FORTRAN structures implied in the finite difference solution as well as the code required for the linking of branches.

The hydrodynamic calculations are completed on a branch by branch basis. Thus, the segment of code in Task 2.2 begins a DO loop over each branch (DO JB=1,NBP) and extracts the upstream [IU] and downstream [ID] segment locations from their respective lists, [CUS] and [DS], for use in the following tasks.

Task 2.2.1: Boundary Concentrations, Temperatures, and Densities

The computations done in this task provide additional boundary condition data to the computation on a branch-by-branch basis. Remember some of the boundary source/sinks were included in the source/sink array [QSS] in Task 2.1. The remaining source/sinks are included in this task and also Task 2.2.3, including upstream and downstream flows and upstream and downstream internal and external heads. These flows enter the computation as momentum sources and need to be included in the water surface elevation computation.

These computations are done on a branch-by-branch basis because the internal head computations depend on having the latest solution to the water surface elevation, especially the elevation for segments at junctions. For example, if branch 2 is connected with the main stem (branch 1) of a reservoir at segment 37, then the hydrodynamic solution for branch 2 needs the boundary head and temperature/constituent profiles at segment 37. Placing these computations in Task 2.2.1 permits the latest available information to be used for each succeeding branch computation.

The computations for external heads or flow boundary conditions could be placed earlier in Task 1.2.1 since the current timestep information comes from user-supplied data files. However, these computations are similar to the internal head computations in that they are branch-specific calculations and are placed here for consistency.

The following code segment illustrates the typical computations in Task 2.2.1:

```
IF (UP_HEAD(JB)) THEN
  IUT = IU-1
  IF (UH_INTERNAL(JB)) THEN
    DO K=KT,KB(IU-1)
      DO JC=1,NAC
        C1(K,IUT,CN(JC)) = C2(K,UHS(JB),CN(JC))
        C2(K,IUT,CN(JC)) = C2(K,UHS(JB),CN(JC))
      END DO
      T1(K,IUT)  = T2(K,UHS(JB))
      T2(K,IUT)  = T2(K,UHS(JB))
      RHO(K,IUT) = RHO(K,UHS(JB))
    END DO
  ELSE IF (UH_EXTERNAL(JB)) THEN
    DO K=KT,KB(IU-1)
      DO JC=1,NAC
        C1(K,IUT,CN(JC)) = CUH(K,CN(JC),JB)
        C2(K,IUT,CN(JC)) = CUH(K,CN(JC),JB)
      END DO
      T1(K,IUT)  = TUH(K,JB)
      T2(K,IUT)  = TUH(K,JB)
      RHO(K,IUT) = DENSITY (T2(K,IUT),SS(K,IUT),DISS(K,IUT))
    END DO
  END IF
END IF
```

Remembering this computation is done within a branch loop, the branch upstream head list [UP_HEAD] is checked to determine if this branch has an upstream head boundary. Assuming it does, it can be either an external (user-supplied head, as for an estuary case) or internal (linked to another branch in the waterbody) head boundary. For the internal case, constituents [C1] and [C2], temperature [T1] and [T2] and density [RHO] profiles at the upstream boundary for the branch are obtained from the junction segment. If it is an external head boundary, the same data are obtained from the arrays [TUH] and [CUH] supplied by the subroutine TIME_VARYING_DATA. In either case,

these boundary profiles are used in the development of momentum terms for the water surface elevation and horizontal velocity calculations.

The following statement

```
IF (.NOT.VIOLATION) THEN
```

ensures these calculations are done only if the timestep did not violate numerical stability requirements and are not repeated if the timestep did.

Task 2.2.2: Momentum Terms

Densities
Density pressures
Horizontal density gradients
Vertical eddy viscosity
Check for density inversions
Shear stresses
Horizontal momentum
Vertical momentum

The computation of the momentum terms follows very closely the finite-difference forms of the momentum equation given in Appendix A. These terms are used both in the water surface elevation solution and in the horizontal velocity field solution. These terms appear in both computations since the solution for the water surface elevation in CE-QUAL-W2 is the continuity equation with the momentum equation substituted for the horizontal velocity terms in that equation. This substitution gives rise to three water surface elevations (central, forward and back) in the equation which is then solved using the tridiagonal algorithm. Thus, the water surface is solved simultaneously with the horizontal velocity field. When the horizontal velocities are later solved algebraically, the solution makes use of the same momentum terms computed in Task 2.2.2.

The computation of densities, density pressures, horizontal density gradients, and vertical eddy viscosities is preparatory to the computation of the terms shown in Appendix A on the right-hand side of Equation (A-13), page A5. Note certain DO loops for [I] are done for [IU] and [ID], and others are done for [IUT] and [IDT]. [IU] and [ID] are the current beginning segment and ending segment for a branch respectively. [IUT] and [IDT] are temporary indices that move the [I] sweep further upstream by a segment or downstream by a segment, respectively, for the case of an internal or external head boundary condition. The presence of a -1 in the terminating index of the sweep indicates a computation is being done at the interface of segments. For example, the computation of densities

```
*********** Densities
          DO I=IU,ID
            DO K=KT,KB(I)
              RHO(K,I) = DENSITY (T2(K,I),SS(K,I),DISS(K,I))
            END DO
          END DO
```

is done only for the segments formally included in the branch. If the branch has an open boundary, the densities in the open boundary segment were computed earlier in Task 2.2.1.

The computation of density pressures (pressures computed without the water surface elevation deviation) needs to include segments that are part of an open boundary specification:

```
*********** Density pressures
          DO I=IUT,IDT
            P(KT,I) = RHO(KT,I)*G*H(KT)
            DO K=KT+1,KB(I)
              P(K,I) = P(K-1,I)+RHO(K,I)*G*H(K)
            END DO
          END DO
```

Contrast the segment indices for this computation with the indices for the previous computation of [RHO(K,I)]. The latter are available at I=IUT and I=IDT for the density pressure computations because they were computed earlier in Task 2.2.1.

Finally, the computation of horizontal density gradients

```
*********** Horizontal density gradients
          DO I=IUT,IDT-1
            DLXRHO    = 1.0/((DLX(I)+DLX(I+1))*RHOI)
            HPG(KT,I) = DLXRHO*(BKT(I)+BKT(I+1))*0.5*(HKT2(I+1)
      .               *P(KT,I+1)-HKT2(I)*P(KT,I))
            DO K=KT+1,KBMIN(I)
              HPG(K,I) = DLXRHO*BHR(K,I)*((P(K-1,I+1)-P(K-1,I))
      .               +(P(K,I+1)-P(K,I)))
            END DO
          END DO
        END IF
```

are done at interfaces at the right hand side of a cell and therefore the computation stops at [IDT]-1.

The vertical eddy viscosity calculation follows the discussion in Appendix A, in which the vertical eddy viscosity has a component due to lateral wind stress, a stress which otherwise would not be included in the longitudinal-vertical computations. The computation also limits the value of the vertical eddy viscosity

to prevent stability violations due to dispersion, $\Delta t < \Delta z^2 / A_z$ (see the variables [AZMXKT(I)] and [AZMAX(K-1)].

The computation of the top [ST] and bottom [SB] shear stresses, the advection of x-direction momentum [ADMX], the diffusion of momentum [DM], and vertical momentum [ADMZ] are computed next and used in the water surface elevation computation and later in the horizontal velocity computation.

Note that [ADMX], [DM], and [ADMZ] are not functions of the timestep [DLT] and need only be computed once. Other variables are timestep dependent and must be recalculated if a timestep violation occurs. As mentioned previously, the logical variable [VIOLATION] controls this process. At the beginning of the hydrodynamic computations, [VIOLATION] has the value "false". If, after the water surface and velocities are updated for the new timestep, the timestep was found to be too large to theoretically maintain numerical stability, then [VIOLATION] is set to ".true.". The water surface elevations and velocities are then recalculated using a smaller timestep. Since [VIOLATION] is now true, then only the code that is timestep dependent is re-executed. See the discussion of Task 2.2.6 (page D26) for more details of the autostepping algorithm.

Task 2.2.3: Water Surface Elevation

Tridiagonal coefficients (D and F)
Boundary tridiagonal coefficients (D and F)
Set boundary surface elevations
Tridiagonal coefficients (A, C, D, and V)
Thomas algorithm for water surface elevation solution
Update surface layer and related variables

The water surface elevation calculation for a given branch uses the longitudinal momentum terms computed in Task 2.2.2. This calculation follows directly from the equations shown in Appendix A.

The first half of this section of code prepares the coefficients necessary for the tridiagonal solution for the water surface elevation. The second half of this section performs the solution and then updates variables related to the new water surface elevation.

The coefficients that need to be prepared are the left-hand side sub-, main- and super-diagonals [A], [V] and [C] and the right-hand side [D]. These terms are identified in Equations (A-20) through (A-22) of Appendix A, page A8.

A common term in these equations is the variable [BHRHO] which is a vertical integral appearing in [A], [C], and [V]. [BHRHO] is calculated at the interfaces between the branch's internal segments as the integral from [KT] to [KBMIN]-1.

At the same time [BHRHO] is being calculated, other vertical integrals are also summed, also at the interfaces but to the layer limit [KB] so any sources/sinks below the [KBMIN] limit can be included. These are [D] and [F], which can also be examined directly in Equations (A-18) and (A-22), in Appendix A, pages A8-A9.

The next code segment augments [D] and [F] to include the boundary data not incorporated in the computation through the hydrodynamic source and sink array [QSS]. These data include upstream inflows [QIN], downstream outflows [QOUT], and upstream and downstream heads, whether internal or external. Note for upstream and downstream heads, an abbreviated set of longitudinal momentum terms [SB], [ST], and [HPG] are included. A more complete expression of the longitudinal momentum terms is not currently in the code. Thus, there is no momentum transfer between branches.

The last head-related task before the final set of coefficients are assembled is to gather the boundary elevations and place them in the appropriate locations for the solution:

```
********* Set boundary surface elevations

        IF (UH_INTERNAL(JB)) Z1(IU-1) = Z1(UHS(JB))
        IF (UH_EXTERNAL(JB)) Z1(IU-1) = EL(KT)-ELUH(JB)
        IF (DH_INTERNAL(JB)) Z1(ID+1) = Z1(DHS(JB))
        IF (DH_EXTERNAL(JB)) Z1(ID+1) = EL(KT)-ELDH(JB)
```

These boundary elevations will then be referenced when solving for the water surface, which is then performed using the Thomas algorithm for the solution of a tridiagonal matrix.

Once the new water surface elevation is computed and placed in [Z1], the surface dependent geometry is updated. This algorithm is similar to the one described in Task 1.4.3 in that the layer in which the water surface resides is computed and water surface elevation dependent geometry is updated.

For each segment in the branch being computed, the new water surface elevation deviation [EL] at [KT]-[Z1] is examined to determine if the elevation is above or below the elevation of the [IKT] layer. Recall the [IKT] layer is the layer in which the water surface elevation for that particular segment actually resides. If the new elevation exceeds the elevation at the top of the [IKT]

layer, [Z1] is modified by spreading the water contained over the [IKT] and [IKT]-1 layers:

```
IF (EL(KT)-Z1(I).GT.EL(IKT(I))) THEN
   DO WHILE (EL(KT)-Z1(I).GT.EL(IKT(I)))
      Z1(I)  = EL(KT)-EL(IKT(I))-(EL(KT)-EL(IKT(I))-Z1(I))
               *(B(IKT(I),I)/B(IKT(I)-1,I))
      IKT(I) = IKT(I)-1
   END DO
```

If the new elevation is less than the elevation at the top of the [IKT] layer, a similar computation is done using geometric data for the [IKT] and [IKT]+1 layers:

```
ELSE IF (EL(KT)-Z1(I).LT.EL(IKT(I)+1)) THEN
   DO WHILE (EL(KT)-Z1(I).LT.EL(IKT(I)+1))
      Z1(I)  = EL(KT)-EL(IKT(I)+1)-(EL(KT)-EL(IKT(I)+1)
               -Z1(I))*(B(IK(I),I)/B(IKT(I)+1,I))
      IKT(I) = IKT(I)+1
   END DO
END IF
```

Once the modified water surface deviations [Z1] are updated, the geometric terms dependent on the water surface elevation are then computed.

Task 2.2.4: Longitudinal Velocities

Pressures
Horizontal pressure gradients
Boundary horizontal velocities
Place inflow according to density
Place inflows according to weighted cell volumes
Horizontal velocities
Corrected horizontal velocities
Head boundary flows

After updating the water surface elevation, horizontal velocities can then be updated. The first step is to compute the pressures and horizontal pressure gradients, which now include the contribution of the newly computed water surface elevation through the surface layer thickness [HKT1] - one of the terms updated at the end of the previous task.

The next step is to compute the boundary horizontal velocities [U]. There are two options for computing upstream flow boundary velocities - place the inflows according to densities or distribute the inflows over the entire upstream segment. For inflows placed according to density, the inflow density is calculated based on temperature and dissolved and suspended solids if the latter two

constituents are modeled. This density is then compared to the density of each cell in the upstream segment until a cell is found with a density greater than the inflow density. A pointer is saved [K] which identifies this layer for the remainder of this computation. Next, the volume of inflow is computed. If the volume of inflow is greater than nine-tenths of the upstream cell volume receiving the inflow, then nine-tenths of the inflow volume is assigned to layer [K] and the remainder is assigned to the layer immediately above. If the computed inflow layer is the surface layer [KT] then the remainder of the inflow is assigned to the layer immediately below [KT]. For inflows distributed over the entire water column, a fraction of the inflow [QINF] is calculated for each upstream cell based on flow weighting and the inflows are apportioned according to the fraction calculated for each cell.

Setting the boundary velocities for the case of downstream flows is done simply on the basis of the outflow specified by layer [QOUT] and [KOUT]. The outflow layer may have been specified by the user or computed by the model using the selective withdrawal routine [SELECTIVE_WITHDRAWAL].

The computation for the head-type boundary velocities is made from the limited set of longitudinal momentum terms computed prior to the surface elevations. Once the boundary horizontal velocities are computed from these terms, e.g.,

```
U(K,ID) = (BHR(K,ID)*U(K,ID)+DLT*(-SB(K,ID)+ST(K,ID)
              -HPG(K,ID)))/BHR(K,ID)
```

the velocities for the entire branch can be computed, based on Equation (A-9) in Appendix A, page A4:

```
U(K,I) = U(K,I)+DLT/BHR(K,I)*(-SB(K,I)+ST(K,I)-ADMZ(K,I)
            +ADMZ(K-1,I)-ADMX(K,I)+DM(K,I)-HPG(K,I))
```

In order to perfectly satisfy continuity, the horizontal velocities [U] are then adjusted based on an overall volume balance for the branch. The overall volume balance is based on the previously completed water surface elevation computations.

The problem to be addressed is the over determination of the basic volume balance in the computation - the volume balance is complete when the water surface elevation computation is finished. However, the code goes on to compute horizontal velocities explicitly for each cell based on the same information used to compute the water surface elevation. This is possible since the hydrodynamic computation is a simultaneous solution of the elevation and velocity computation. The code then computes the vertical velocities from the continuity equation, integrating at each segment from the bottom up.

This single pass through all the equations inevitably results in some inconsistencies. In Version 1.0, these inconsistences showed up in the vertical velocities at the bottom of the surface cells. The inconsistency was these velocities did not perfectly balance the change in storage in the top cells (since the water surface lies within these top cells, their volume changes). This problem was addressed by maintaining a separate vertical velocity [WKT] for these cells computed from the top cell volume balance rather than from integrating the continuity equation from the bottom up, as is done for the ordinary vertical velocities. This approach did not solve the problem, however, since the constituent equation continued to have a slight volume error.

The approach taken here, which results in volume balances to machine accuracy, is to adjust the horizontal flows after they have been explicitly computed using a volume balance based on the water surface elevation. This algorithm is discussed in detail below.

There is yet another approach to the volume balance problem. One should recognize that although the computation for elevations and velocities is simultaneous, certain terms in the elevation solution depend on the magnitude of the velocities, which are not known until the water surface elevation is computed. In fact, the theoretically correct approach is to iterate through the [Z]-[U]-[W] computation until a perfect water balance is attained. This balance can be achieve in about four iterations. However, the cost is to increase the time devoted to the hydrodynamic computation. The compromise adopted here results in both perfect mass and constituent balances.

The velocity adjustment procedure is based on computing vertically integrated flows at each segment [Q(I)], which are based on the recently solved horizontal velocities:

```
Q(IU-1) = U(KT,IU-1)*BHRKT1(IU-1)
DO K=KB(IU),KT+1,-1
  Q(IU-1) = Q(IU-1)+U(K,IU-1)*BHR(K,IU-1)
END DO
QC(IU-1) = Q(IU-1)
DO I=IU,ID
  BHRSUM = 0.0
  IF (I.EQ.ID.AND.DN_FLOW(JB)) THEN
    Q(I)     = 0.0
    QSSUM(I) = 0.0
    DO K=KT,KB(I)
      QSSUM(I) = QSSUM(I)+QSS(K,I)
    END DO
    DO JO=1,NOUT(JB)
      K = KOUT(JO,JB)
      IF (K.GE.KT) THEN
        BHRT = BHR(K,I)
        IF (K.EQ.KT) BHRT = BHRKT1(I)
        IF (U(K,I).NE.0.0) BHRSUM = BHRSUM+BHRT
        Q(I) = Q(I)+U(K,I)*BHRT
```

```
      END IF
    END DO
  ELSE
    BHRSUM    = BHRKT1(I)
    Q(I)      = U(KT,I)*BHRKT1(I)
    QSSUM(I) = QSS(KT,I)
    DO K=KBMIN(I),KT+1,-1
      BHRSUM    = BHRSUM+BHR(K,I)
      Q(I)      = Q(I)+U(K,I)*BHR(K,I)
      QSSUM(I) = QSSUM(I)+QSS(K,I)
    END DO
  END IF
```

The variable [Q] is initialized at the upstream segment [IU]-1 and then vertically and longitudinally integrated. At the same time, any sources/sinks [QSS(K,I)] are accounted for. The logic within the DO loop allows the computation to account for either downstream flow or downstream head conditions.

A similar computation is done for the corrected vertically integrated flows [QC(I)]. These differ from the vertically integrated flows [Q] in that the change in storage over the timestep, [BHKT2] - [BHKT1], is added. This permits the adjustment of the horizontal flows [U] by adding or subtracting to them the amount necessary for perfect volume balances through the entire [Z]-[U]-[W] pass:

```
QC(I) = QC(I-1)+DLX(I)/DLT*(BHKT2(I)-BHKT1(I))+QSSUM(I)
IF (I.EQ.ID.AND.DN_FLOW(JB)) THEN
  DO JO=1,NOUT(JB)
    K = KOUT(JO,JB)
    IF (K.GE.KT.AND.U(K,I).NE.0.0) THEN
      U(K,I) = U(K,I)+(QC(I)-Q(I))/BHRSUM
    END IF
  END DO
ELSE
  DO K=KBMIN(I),KT,-1
    U(K,I) = U(K,I)+(QC(I)-Q(I))/BHRSUM
  END DO
END IF
END DO
```

Task 2.2.5: Vertical Velocities

Calculation of the vertical velocities [W] completes the hydrodynamic calculations and, as shown in the previous section, completes the perfect volume balance. They are computed from continuity, beginning at the bottom cell of each segment using the known (and adjusted) horizontal velocities [U] and bottom vertical velocities [W] (always zero for the bottom cell) to compute the vertical velocity at the top of each cell. At the end of this task, hydrodynamics have been computed for each branch pending the autostepping algorithm that determines if there has been a timestep violation.

Task 2.2.6: Autostepping

Task 2.2.6 was referred to when discussing the logical variable VIOLATION. The purpose of this task is to examine the current timestep [DLT] to determine if it violates the hydrodynamic numerical stability criteria in the finite difference solution.

The following computations are done for each active cell in the grid. The surface layer thickness for each cell is computed based on the newly computed water surface elevation deviation and a warning message is written if the height in any segment is less than zero. This is a severe error and typically arises when a large surface wave is generated which causes the water surface to extend into layer [KT] + 1 over one timestep. The solution to this problem is to add/subtract layers immediately after computing the new water surface elevations [Z1]. This will be fixed in Version 3.0.

Next, the stability limits based on the internal gravity wave speed [CELRTY], and the advection/diffusion criteria, [TAU1], [TAU2], and [QTOT], are calculated. The criteria are given in equation (D-1).

$$\Delta t \ \leq \ \cfrac{1}{2\left[\dfrac{A_x}{\Delta x^2} + \dfrac{A_z}{\Delta z^2}\right] + \dfrac{Q}{V} + \cfrac{\sqrt{\dfrac{\Delta\rho}{\rho}\dfrac{gH}{2}}}{\Delta x}} \qquad\text{(D-1)}$$

where

Δt = timestep, *sec*
A_x = longitudinal eddy viscosity, $m^2\ sec^{-1}$
A_z = vertical eddy viscosity, $m^2\ sec^{-1}$
Q = total flow into or out of a cell, $m^3\ sec^{-1}$
V = cell volume, m^3
g = gravitational acceleration, m sec^{-2}
H = maximum waterbody depth, m
ρ = water density, $kg\ m^{-3}$
$\Delta\rho$ = surface to bottom water density difference, $kg\ m^{-3}$

The calculated maximum timestep [DLTCAL] is compared to the current maximum calculated timestep [CURMAX]. If [DLTCAL] is less than [CURMAX], then [CURMAX] is assigned the value of [DLTCAL], the segment [ILOC] and layer [KLOC] pointers containing the limiting timestep location are updated, and the computations proceed for the remainder of the grid. After the computations for the entire grid are completed, then [CURMAX] will contain the maxi-

mum computed value of the timestep necessary to maintain hydrodynamic stability with [ILOC] and [KLOC] pointing to the cell which produced this value. Additional coding keeps track of the minimum timestep during a simulation [MINDLT] and its location [KMIN] and [IMIN].

The calculated maximum timestep [CURMAX] is then compared to the actual timestep used in the water surface elevation and velocity calculations. Also included is a comparison to the minimum timestep [MINDLT] specified in the control file (see page C4). [MINDLT] is included to prevent the timestep from becoming too small for the run to be economical, but care must be taken in its use. It is possible to violate hydrodynamic stability if [MINDLT] is set to high. A warning message is output to the warning file [WRNFN] if the timestep drops to the minimum value.

If the calculated maximum timestep [CURMAX] is less than the timestep used in the hydrodynamic calculations and greater than the user-specified minimum timestep, then the actual timestep to be used in the recalculation of the water surface and velocities is computed by multiplying [CURMAX] by the timestep fraction [DLTF] specified by the user (see page C7). There is a threefold reason for multiplying [CURMAX] by [DLTF]. First, [CURMAX] may be on the edge of numerical stability. Multiplying [CURMAX] by [DLTF] is a safety factor. Second, using only a fraction of [CURMAX] reduces the number of timestep violations as the computations proceed. For example, if [DLTF] is set to 0.9, then [CURMAX] calculated during the next iteration of the code can decrease by as much as 10% without causing a timestep violation. Finally, the criteria for numerical stability used in the autostepping algorithm ensure the hydrodynamic stability criteria are met. The model can still become unstable during the water quality transport calculations if more mass is removed from a cell over a timestep via the kinetic source/sink term [CSSK] than exists in the cell.

If the timestep [DLT] is less than the minimum timestep, then the date and timestep are sent to the warning output file [WRNFN] to alert the user the computations may be unstable at this point in the simulation, and the timestep is then set to [DLTMIN]. The current maximum timestep [CURMAX] is then reset to the maximum timestep [DLTMAX] specified on the **Timestep Control Card** (see page C4). Finally, saved values of the water surface elevation deviation [SZ1], minimum layer number [SIKT], and velocity fields, [SU] and [SW], are retrieved and placed in their corresponding arrays. The hydrodynamic source and sink array [QSS] is reinitialized to zero since the flows between branches are lagged in time and thus timestep dependent. The computation is then returned to the entry point (10010 CONTINUE) where only the timestep dependent calculations are repeated. This is one of the few places where a GO

TO statement is used in the code because it is one of the few instances where the coding is simplified by using it.

Task 2.3: Temporal Balance Terms and Temperatures

Surface heat exchange
Ice present
Heat balance at air-ice interface
Solar radiation attenuation
Ice growth at ice-water interface
Ice melt at ice-water interface
Total ice thickness
External heat sources/sinks and total inflow/outflow
Horizontal advection and diffusion multipliers
Vertical advection multipliers
Transport heat
Vertical advection and implicit diffusion
Tridiagonal solution

After evaluation of the elevation and velocity fields and checks to ensure numerical stability, the program proceeds to the transport computations. The transport computations are identical for temperature and each constituent except for the differing sources/sinks. Sources/sinks are represented by the right-hand side of Equation (A-2) in Appendix A. An inefficient FORTRAN construction of the transport computations would repeat the entire sequence performed for the first computation for each successive computation. However, as noted in Appendix A, there are several parts of the transport computation that can be saved after temperature transport for use later in computing the transport of constituents. One of these parts was already noted in Task 1.4.3 when the spatially invariant transport interpolation multipliers were computed prior to the start of the model's main time loop [SF2L...SF14L and SF2V...SF11V].

During the transport of heat, spatially invariant coefficients are computed and saved to be used later in constituent transport. These include the longitudinal [AD1L], [AD2L], and [AD3L] and vertical [AD1V], [AD2V], and [AD3V] advection multipliers.

The transport computation includes both the upwind and QUICKEST formulations. The QUICKEST formulation is the preferred option, but since the upwind form is a subset of QUICKEST, the old transport scheme is still retained for those who feel uncomfortable with change. An input switch [SLTC] on the **Transport Scheme** card allows the user to select either method (see page C19).

The transport of heat also differs from the constituent computations in that the sources/sinks are, for the most part, evaluated in the main code, rather than in subroutines. Further, the computation of ice thickness, a parameter closely related to water temperature, is computed at the same time as the transport of heat.

The user may chose between the linearized surface heat computation, which uses the coefficient of surface heat exchange and equilibrium temperature, and the term by term heat budget, which computes the individual heat exchange terms. If the latter has been selected, two subroutines are called at the beginning of Task 2.3: HEAT_EXCHANGE, which computes incident solar radiation, surface heat exchange, and equilibrium temperature, and RADIATION which computes absorbed solar radiation and long-wave atmospheric radiation. Surface heat exchange and equilibrium temperature are always needed for ice computation.

Assuming surface heat exchange is to be included in the computation at all [NO_HEAT], the surface heat exchange computation consists of either the linearized surface heat exchange with attenuated through the water column. Note a third heat exchange subroutine is called for the term-by-term heat budget [SURFACE_TERMS]. This subroutine computes the three surface heat exchange components dependent on the water surface temperature. The presence of these three terms is the main difference between the two approaches. In either case, solar radiation is attenuated through the water column. Note neither of the surface heat exchange computations are done if ice cover is present.

The ice cover computation includes two input parameters used during calibration - the temperature at which ice is permitted to form [ICET2] and the minimum ice thickness [ICEMIN]. The first part of the ice computation converts these parameters into the logic control variables [ALLOW_ICE] and [ICE_IN]. The ice calculation itself can be done either of two ways. The first option, [DETAILED_ICE], is based on individual heat balances and the air-ice-water interfaces and requires a separate computation of initial ice thickness which is triggered by a computed water temperature less than zero:

```
IF (T2(KT,I).LT.0.0) THEN
  IF (INIT(I).EQ.0) THEN
    ICETH2 = -T2(KT,I)*RHO(KT,I)*CP*HKT2(I)/(RHOICE
             *RL1)
    IF (ICETH2.LT.0.005) THEN
      ICETH2  = 0.0
      INIT(I) = 0
    ELSE
      TSS(KT,I) = TSS(KT,I)-T2(KT,I)*RHO(KT,I)*CP
                  *HKT2(I)*B(IKT(I),I)/4.186E6/DLT
                  *DLX(I)
      INIT(I)   = 1
```

```
                      END IF
                    END IF
```

The ice thickness [ICETH2] is computed as the amount of heat that would have gone into ice formation. If this thickness is less than half a centimeter, it is ignored (assuming wind breakup and mixing of this thin ice). If it is thicker, then the temperature heat balance is corrected and the initial ice flag [INIT] is set to 1 for this segment.

On time iterations after ice formation, the ice logical variable [ICE] is true, and surface heat exchange for the air-ice interface is computed using the linearized surface heat exchange computations. This procedure is iterative, since the ice temperature must be computed and surface heat exchange recomputed until a solution is found:

```
                 ICOUNT = 0
                 TICE   = TAIR
10040            CONTINUE
                 ICOUNT = ICOUNT+1
                 IF (ICOUNT.GT.2000) GO TO 10050
                 CALL SURFACE_TERMS (TAIR,TDEW,WIND,TICE,RB,RE,RC)
                 RN(I) = RS*(1.0-ALBEDO)*BETAI+RAN-RB-RE-RC

****************** Heat balance at air-ice interface

                 DEL = RN(I)+RK1*(RIMT-TICE)/ICETH(I)
                 IF (ABS(DEL).GT.1.0) THEN
                   TICE = TICE+DEL/500.0
                   GO TO 10040
                 END IF
10050            CONTINUE
```

Following this computation, solar radiation attenuation through the ice, ice growth and melt at the ice-water interface, and total ice thickness are then computed.

The alternate, simple ice computation is:

```
            HIA      = 0.2367*CSHE/5.65E-8
            ICETH(I) = ICETH(I)+DLT*((RIMT-ET)/(ICETH(I)/RK1+1.0
       .                 /HIA)-(T2(KT,I)-RIMT))/(RHOICE*RL1)
            ICETH(I) = MAX(ICETH(I),0.0)
            ICE(I)   = ICETH(I).GT.0.0
            IF (ICE(I)) THEN
              TSS(KT,I) = TSS(KT,I)+2.392E-7*(RIMT-T2(KT,I))
       .                  *B(IKT(I),I)*DLX(I)
```

This computation is based on the heat balance over the entire ice thickness.

Similar to the boundary inflow and outflow computations, heat from inflows and outflows are included in the temperature source and sink array [TSS]. At

this time, information is accumulated that is used in determining the computations overall volume balance. The variables [VOLEV], [VOLPR], [VOLTR], [VOLDT], [VOLWD], [VOLIN], [VOLOUT], [VOLUH], [VOLDH] keep track of the volume added or subtracted over the timestep by the evaporation, tributary, distributed tributary, withdrawal, inflow, outflow, and upstream and downstream head processes.

Furthermore, the temperature source and sink arrays [TSS] are updated for these same processes. The augmentation of [TSS] for the head boundary conditions notes that these interchanges between branches are not automatically calculated when flows leave a particular branch.

The last steps in this task are to calculate the horizontal and vertical advection and diffusion multipliers and the transport of heat. These advective multipliers are independent of the constituent being transported and are computed prior to the computation of the first constituent, temperature, so they are available for that computation as well as each succeeding computation. The reader should consult Appendix A, page A10 for an overview of the transport computation as well as the rationale for the preparation of the multipliers at this stage. The advective multipliers are shown as Equation (A-25).

The advective multipliers become part of the advective fluxes that must be done for each constituent. Since temperature is always computed, it is included in this task rather than in the constituent transport, Task 2.4. An examination of the temperature computation (marked "Transport heat" in the code) shows the general features of the QUICKEST computation.

The first part of the QUICKEST computation is completed with the solution for the new temperature [T1] based only on horizontal advective and dispersive fluxes and boundary fluxes (and vertical fluxes depending on the value of [THETA]):

```
DO JB=1,NBP
  IU = CUS(JB)
  ID = DS(JB)
  DO I=IU,ID
    T1(KT,I) = (T2(KT,I)*BHKT2(I)/DLT+(TADL(KT,I)*BHRKT1(I)
.               -TADL(KT,I-1)*BHRKT1(I-1))/DLX(I)+(1.0-THETA)
.               *TADV(KT,I)*BB(KT,I)+TSS(KT,I)/DLX(I))*DLT
.               /BHKT1(I)
    DO K=KT+1,KB(I)
      T1(K,I) = (T2(K,I)*BH(K,I)/DLT+(TADL(K,I)*BHR(K,I)
.                 -TADL(K,I-1)*BHR(K,I-1))/DLX(I)+(1.0-THETA)
.                 *(TADV(K,I)*BB(K,I)-TADV(K-1,I)*BB(K-1,I))
.                 +TSS(K,I)/DLX(I))*DLT/BH(K,I)
    END DO
```

Note there is a slightly different form of this equation for the top layer which uses geometric terms based on water surface elevations that vary from iteration to iteration and are stored separately.

In the second part of the transport scheme, vertical diffusion is calculated implicitly. The second part of the transport scheme is solved implicitly with the vertical temperature dependent terms moved to the left-hand side of the equation to provide the three tri-diagonal coefficients. Thus, a fully explicit, [THETA]=0, or fully implicit, [THETA]=1, vertical advection can be specified in the solution. The Thomas algorithm is used for the final solution for temperature.

Task 2.4: Constituents

Internal sources/sinks
External sources/sinks
Transport constituents
Horizontal advection and diffusion terms
Vertical advection terms
Transport constituents
Crank-Nicholson vertical advection and implicit diffusion

The outline of this task is similar to Task 2.3, except kinetic sources/sinks for the water quality parameters need to be computed via the kinetic subroutine calls, and the computation proceeds over multiple constituents. Most transport terms have already been computed during temperature transport (Task 2.3).

The logical variable [UPDATE_KINETICS] is used to control whether the kinetics subroutines are called at a given timestep. This logic variable is determined from the frequency of kinetic updates [FREQUK] specified on the **Constituent Computations** card (see page C69). The subroutines RATE_MULTIPLIERS and DECAY_CONSTANTS are called first. RATE_MULTIPLIERS computes the temperature dependent rate multipliers and DECAY_CONSTANTS computes the water quality rate constants used in the kinetic formulations.

Following these computations, sources/sinks due to boundary inflows and outflows are computed in a manner similar to those in heat transport. The actual transport of constituents follows closely the transport of heat except many of the coefficient arrays have already been computed. A comparison of the two computations will readily show the differences.

Task 2.5: Layer - Segment Addition and Subtraction

Determine water surface minimum height
Initialize variables in new layer
Upstream active cell
Add segments
Initialize variables in subtracted layer
Initialize variables in new layer
Upstream active cell
Subtract segments

After the hydrodynamic and transport computations are performed for the entire grid, new values for water surface elevation, velocity, temperature, and constituent fields exist throughout the finite difference grid representation of the waterbody. At this point, water surface elevations are examined to determine if layers should be added or subtracted. The code calculates the minimum height of the water surface over the entire grid [ZMIN] which is then used to determine if layers need to be added or subtracted.

While [ZMIN] extends less then 0.8 of the way into the next higher layer [KT]-1 or extends less then 0.6 of the way into the current surface layer [KT], no action is taken. However, when the minimum water surface extends above the upper limit, a layer is added to better resolve the current top layer. Note the water surface position is not changed, but the surface layer is divided into two layers. This layer addition may in turn allow the addition of upstream segments to the active computational grid for a particular branch based on the requirement that there must be at least two active layers in an active segment. The active grid therefore expands upward and upstream in response to increasing water surface elevations.

Conversely, when the current surface layer is less than 40 percent full at the segment where the water surface elevation deviation is lowest [ZMIN], then the current surface layer is incorporated into the next lower layer. This requires the examination of the current upstream boundary segment [CUS] to determine whether segments need to be subtracted to fulfill the requirement of two active layers at each active segment.

[ZMIN] is then used in the setting of two logical variables for layer addition [ADD_LAYER] and subtraction [SUB_LAYER]. The evaluation of these logical variables express the rules noted earlier for layer additions and subtractions:

```
ADD_LAYER = ZMIN.LT.-0.80*H(KT-1).AND.KT.NE.2
SUB_LAYER = ZMIN.GT.0.60*H(KT)
```

The remainder of this task is divided into the code for adding a layer and the code for subtracting a layer. When adding a layer, the existing layer is divided into two layers - one completely full and the other (the new surface layer) partially full.

Geometric terms for the new layer are recomputed for each branch and each segment and the temperatures and constituent concentrations computed for the previous surface layer [KT]+1 are assigned to the new surface layer:

```
DO JB=1,NBP
  IU = CUS(JB)
  ID = DS(JB)
  DO I=IU-1,ID+1
    Z1(I)     = H(KT)+Z1(I)
    U(KT,I)   = U(KT+1,I)
    W(KT,I)   = W(KT+1,I)*(BB(KT+1,I)/BB(KT,I))
    HKT1(I)   = H(KT)-Z1(I)
    BHKT1(I)  = BHKT1(I)-BH(KT+1,I)
    BKT(I)    = BHKT1(I)/HKT1(I)
    T1(KT,I)  = T1(KT+1,I)
    DO JC=1,NAC
      C1(KT,I,CN(JC))   = C1(KT+1,I,CN(JC))
      CSSK(KT,I,CN(JC)) = CSSK(KT+1,I,CN(JC))
    END DO
  END DO
  DO I=IU-1,ID
    BHRKT1(I) = (BHKT1(I)+BHKT1(I+1))*0.5
  END DO
```

Since this procedure simply breaks an existing layer into two, the temperatures and constituent concentrations from the previous single layer are assigned to the new layer. Geometry updates are done for upstream and downstream head conditions and related variables. For an upstream head boundary, these include the total cross-section area at the head boundary [BHSUM], and flow [QUH1], temperature [TSSUH1], and constituent mass fluxes [CSSUH1]. Similar updates are done for the downstream head condition. With the resetting of the horizontal and vertical eddy viscosity [DX] and [AZ], the layer addition for the case of no upstream cell additions is complete for the given branch.

At this point in the layer addition algorithm, the upstream segments are examined to determine if the layer addition allows additional upstream segments to be incorporated into the active grid. This logic is accomplished by examining the number of layers in the candidate segments [KB]-[KT] based on the new surface layer location and setting a new, temporary upstream segment limit [IUT]:

```
I = US(JB)
DO WHILE (KB(I)-KT.LT.1.AND.I.LT.DS(JB))
  I = I+1
END DO
IUT = I
```

If the new upstream segment [IUT] is not the same as the current upstream segment [IU], then the grid is expanded to incorporate the new segments which meet the two active layer minimum criteria. This procedure is straightforward. Note when the process of initializing the newly added segments is complete, the new upstream segment limit [IUT] is transferred to the current upstream segment array [CUS]. The temperature and constituent concentrations used to set values in the new segments come from the previous current upstream segment. This procedure is different from layer additions where the concentrations in the new layer are unambiguous since they come simply from the divided current layer. Here, upstream concentrations are *estimated* from the previous current upstream segment concentrations. An alternate procedure would be to initialize the new active segments to the inflow temperatures [TIN] and concentrations [CIN]. To complete the DO WHILE loop for layer addition, a new [ZMIN] is computed and the logical variable [ADD_LAYER] is reset. It is possible for the new water surface elevation to increase sufficiently that another layer needs to be added. This is rare, but possible.

When subtracting a layer, a similar process is followed. The main difference is temperatures and constituent concentrations from the old surface layer are mixed into the new surface layer based on volume-weighted concentrations thus maintaining mass balance.

```
T1(KT,I) = (T1(KT-1,I)*(BHKT1(I)-BH(KT,I))
              +T1(KT,I)*BH(KT,I))/BHKT1(I)
```

When the subtraction of a layer causes the subtraction of one or more segments, the temperatures and concentrations in those segments are reset to zero.

The layer and segment subtraction DO WHILE loop ends with a recomputation of [ZMIN] and the resetting of the logical variable [SUB_LAYER]. Again, it is rare that more than one layer will need to be subtracted, but still possible.

Task 2.6: Balances

Water quality modeling is fundamentally a process of keeping track of mass - through boundary sources/sinks and internal transformations. An absolute requirement of the solution is the finite difference representation of the water-body, the transport solution technique, and the kinetic transformations conserve mass. Thus, any acceptable water quality model must be shown to be conservative - including water, heat, and constituents.

Volume balances are computed when the logical variable [VOL_BALANCE] is set to true via the [VBC] variable on the **Calculations** card in the control file (see page C12). The algorithm compares the spatial change in volume

[VOLSBR] based on changes in the water surface elevation for each branch to the initial volumes plus the net inflow/outflow during the simulation [VOLTBR]. The spatial change is computed by summing the changes in volume in the surface layer for each timestep [DLVOL]. This spatial integral is thus dependent on the details of the computation as it directly reflects the solution to the surface elevation equation as well as any manipulations of the grid through layer and segment additions and subtractions. The change in the temporally integrated volume [VOLTBR] is a direct result of the boundary conditions which affect volume (ie., inflows/outflows, branch exchanges, precipitation, and evaporation).

If the difference between the spatially and temporally integrated volumes exceeds the volume tolerance [VTOL] (set to 100 m^3 in the code) a warning is written to the warning file [WRNFN]. During the implementation of a new algorithm or some other extension of the coding, an error in the volume balance indicates an error in the algorithm. Errors are also produced if numerical stability requirements are violated. Diagnosing this error can be accomplished by monitoring the balance. Typical volume balance errors are 1 m^3 out of $1x10^6$ m^3 on a 32 bit machine.

Similar balances are kept for each constituent under control of the logical variable MASS_BALANCE. Here, the spatial integral is determined by examining each cell in each branch and the temporal integral by accessing the constituent source and sink arrays. Typical mass balance errors are 1g out of $1x10^6$g on a 32 bit machine.

Task 2.7: Update Variables for Next Timestep

The variables representing the water surface elevation and derived surface elevation geometry, temperature, and constituents exist at two time levels. At the start of the integration loop, current values (timestep n) are located in arrays suffixed with a "2". As new values (timestep n+1) are computed, they are placed in arrays suffixed with a "1". At the end of the integration loop, new values are placed in arrays suffixed with a "2" in preparation for the beginning of the next timestep integration.

The saved arrays are also updated here. These arrays keep track of the variables used on a second iteration through the time loop in the event of a timestep violation. Any negative concentrations in the constituent array [C2] are eliminated so negative concentrations are not passed into kinetics subroutines. The negative concentrations are placed in the saved constituent array [C1S] used in the transport computations. This ensures mass balances are maintained. For kinetics to act again upon a constituent whose concentration is negative, suffi-

cient mass must be transported into a cell or produced from kinetic interactions during the simulation.

Task 2.7 finishes by updating all timestep dependent variables. These include the number of iterations [NIT] and the simulation time [JDAY]. The logical variable signalling the end of the simulation [END_RUN] is also reset for use in the time loop (DO WHILE (.NOT.END_RUN)). Variables related to the variable timestep algorithm are also updated. In particular, the timestep [DLT] is reset as the maximum of the user specified minimum [DLTMIN] and as a user specified fraction of the current maximum [DLTMAX].

Task 2.8: Output Results

Snapshots
Vertical profiles
Velocity vectors
Contours
Time series
Restart

The final task before going to the next integration timestep is to write results to the various output files opened in Task 1.5 (see page D14). The results generated by CE-QUAL-W2 are longitudinal/vertical grids of velocities, temperatures, constituents, and longitudinal profiles of surface elevations produced at each timestep. In order to examine in detail portions of what would be an immense record for a year-long simulation, several types of summaries are available. The most widely used is the snapshot, which is a longitudinal/vertical grid for selected segments at some useful frequency (e.g., every two weeks for a simulation period of one year). Other summaries available are values over time of a particular parameter at a specific location. An example would be outlet release temperatures. Also, vertical profiles at user specified segments may be output for plotting. This output is used primarily to compare computed and observed values. Finally, grids of velocities at a given frequency may be output for vector plots of circulation fields and grids of constituent concentrations may be output for contour plots.

The snapshot date [SNPD] and frequency [SNPF] variables set in Task 1.4.2 are used to determine if it is time to print a new set of snapshots:

```
IF (SNAPSHOT) THEN
  IF (JDAY.GE.NXTMSN.OR.JDAY.GE.SNPD(SNPDP+1)) THEN
    IF (JDAY.GE.SNPD(SNPDP+1)) THEN
      SNPDP  = SNPDP+1
      NXTMSN = SNPD(SNPDP)
    END IF
    NXTMSN = NXTMSN+SNPF(SNPDP)
```

If NXTMSN has been encountered, NXTMSN is updated and output is sent to the snapshot file [SNPFN]. Much of the code in this section involves writing information for the snapshot header. The elevations, velocities and constituent concentrations themselves are output by the subroutine PRINT_GRID.

The logic for determining when output is sent to the other output files is identical to that of the snapshot file. The reader can examine the specific information written to each file.

Logic for restart output is similar to the logic for snapshots. However, each restart output is saved to a separate file. The inability of FORTRAN to eliminate blanks in character names requires the logic shown here for concatenating a julian day to the file name "rso". The binary write to these files are identical to the reads shown in Task 1.3.

Task 3: End Simulation

Profile FORMATs
Snapshot FORMATs
Run time information FORMATs
Time series FORMAT's
Run time warning FORMATs
Run time error FORMATs
Contour plot FORMATs

The computation is ended after the user-specified ending time is reached (see Task 1.3). All open files are closed.

Subroutine TIME_VARYING_DATA

Subroutine TIME_VARYING_DATA reads all time-varying boundary conditions required by the model during a simulation. The subroutine opens required input files and reads in boundary conditions at appropriate times. The system for reading these files is best explained by examining a particular boundary input in detail.

An upstream inflow and its temperature and constituent concentrations are the most commonly used time-varying boundary condition data. Variables associated with the input of these data are the logical variable [UP_FLOW], the FORTRAN unit numbers [INQ], [INT] and [INC], and the filenames [QINFN], [TINFN] and [CINFN]. Each variable is dimensioned to the number of branches in the waterbody [NBP] so each branch can have a separate inflow file.

The logical variable [UP_FLOW] is set to "true" if the upstream boundary condition variable [UHS] is set to 0, which specifies an external inflow boundary condition. [UP_FLOW] is then used to access the code that initializes the unit numbers and opens the associated files:

```
IF (UP_FLOW(JB)) THEN
  INQ(JB) = UNIT
  UNIT    = UNIT+1
  INT(JB) = UNIT
  UNIT    = UNIT+1
  OPEN (INQ(JB),FILE=QINFN(JB),STATUS='OLD')
  OPEN (INT(JB),FILE=TINFN(JB),STATUS='OLD')
  READ (INQ(JB),1000)
  READ (INT(JB),1000)
  IF (CONSTITUENTS) THEN
    INC(JB) = UNIT
    UNIT    = UNIT+1
    OPEN (INC(JB),FILE=CINFN(JB),STATUS='OLD')
    READ (INC(JB),1000)
  END IF
END IF
```

Unit numbers corresponding to a particular inflow files are computed and stored in arrays (ie., [INT] for the inflow temperature file for branch JB) and may vary from one application to the next depending upon which boundary conditions are included in the application. This code segment also illustrates the use of a related logical variable, CONSTITUENTS, that, when set to "true", reads in time-varying concentrations for each constituent being modeled.

The variable [UP_FLOW] is also used to read the opened file. In the following code segment, two sets of time-varying inflow data and the date associated with each is read and assigned to the inflow variable [QIN] used in the hydrodynamic computation:

```
IF (UP_FLOW(JB)) THEN
  IF (JDAY.GE.NXQIN1(JB)) THEN
    DO WHILE (JDAY.GE.NXQIN1(JB))
      NXQIN2(JB) = NXQIN1(JB)
      QIN(JB)    = QINNX(JB)
      QINO(JB)   = QINNX(JB)
      READ (INQ(JB),1020) NXQIN1(JB),QINNX(JB)
    END DO
  END IF
  NXTVD = MIN(NXTVD,NXQIN1(JB))
```

The algorithm is based on always having two sets of inflow data in memory. Dates for these two sets must straddle or fall on the current simulation time [JDAY]. [NXQIN2] is the time associated with the inflow data immediately prior to or on [JDAY], and [NXQIN1] is the time associated with the next inflow date. On the first call to TIME_VARYING_DATA, statements lying within the range IF (JDAY.GE.NXQIN1(JB)) THEN ... END IF are used to

read a set of time-varying inflow data up until [JDAY] is less than [NXQIN1] - that is, until the end point for the straddle exceeds [JDAY]. This procedure includes exchanging new data set for old so a chronological sequence is maintained - the beginning point for the straddle, [NXQIN2], is set to the previous end point, the values for [QIN] and [QINO] are set to the previous end point values and new end point values are read. The inflow array [QIN] is used directly in the hydrodynamic solution. The old inflow value [QINO] is used by the interpolation subroutine.

On every succeeding call to TIME_VARYING_DATA, a check is made to see if the current date [JDAY] exceeds the date for updating inflows. If it does, data is exchanged and a new set is read, as described previously. If not, the value of [QIN] is correct and nothing additional need be done.

The subroutine also keeps track of the time until the next time-varying data *of any kind* is required to be read by use of the variable [NXTVD]. TIME_VARYING_DATA is only called by the main code when [JDAY] equals or exceeds [NXTVD].

Another feature of TIME_VARYING_DATA is its ability to read only those constituent concentrations the user has specified are available for a particular type of inflow (upstream inflow, tributary, distributed tributary or precipitation).

The list of constituents for which inflow concentrations are available [INCN] is used to select which constituent concentrations are read from the inflow constituent file. Task 1.4.2 in the initialization section of the code previously determined the number of active inflow constituents and their numbers based on the variable [INACC] located on the **Inflow Active Constituent Control** card (see page C75) card in the control file.

```
********** Inflow constituent concentrations

          IF (CONSTITUENTS) THEN
           IF (JDAY.GE.NXCIN1(JB)) THEN
             DO WHILE (JDAY.GE.NXCIN1(JB))
               NXCIN2(JB) = NXCIN1(JB)
               DO JC=1,NACIN
                 CIN(INCN(JC),JB)  = CINNX(INCN(JC),JB)
                 CINO(INCN(JC),JB) = CINNX(INCN(JC),JB)
               END DO
               READ (INC(JB),1030) NXCIN1(JB),(CINNX(INCN(JC),JB),
    .                              JC=1,NACIN)
             END DO
           END IF
           NXTVD = MIN(NXTVD,NXCIN1(JB))
          END IF
         END IF
```

The alternative to this procedure would be to ask for a constituent concentration for every constituent being simulated, regardless of whether these data were available. External head boundary data are handled differently. If an external head boundary has been specified, then the user must supply an external boundary profile for each active constituent.

The final section of code in TIME_VARYING_DATA allows the user to conveniently turn off any or all of the external forcing functions associated with the time-varying data. This procedure is useful in debugging problems due to incorrect or extreme values of, for example, wind or inflow rates. This section of code is activated by the variables [WINDC], [QINC], [QOUTC], and [HEATC] on the **Dead Sea** card. The case of turning all these forcing functions off is called the dead sea case because no motion results. Without this feature, the user would have to construct a debugging data set in which each time-varying input would be set to zero.

Subroutine INTERPOLATE_INPUTS

TIME_VARYING_DATA supplies boundary data at the correct time, and INTERPOLATE_INPUTS linearly interpolates the data which otherwise would be supplied as a step function. Each boundary condition data type may be individually interpolated. The **Interpolation** card (see page C14) may be examined to identify the time-varying boundary data which can be interpolated. Continuing with the example of the upstream inflows used in the discussion of TIME_VARYING_DATA, it can be seen from the following code fragment the interpolation is based on the fraction of time between the previous inflow value and the next inflow value [QRATIO]. Different ratios are used for the temperature and constituent values since these data can occur at different frequencies.

```
IF (UP_FLOW(JB)) THEN
  IF (INTERP_INFLOW) THEN
    QRATIO = (NXQIN1(JB)-JDAY)/(NXQIN1(JB)-NXQIN2(JB))
    TRATIO = (NXTIN1(JB)-JDAY)/(NXTIN1(JB)-NXTIN2(JB))
    IF (CONSTITUENTS) THEN
      CRATIO = (NXCIN1(JB)-JDAY)/(NXCIN1(JB)-NXCIN2(JB))
    END IF
    QIN(JB) = (1.0-QRATIO)*QINNX(JB)+QRATIO*QINO(JB)
    TIN(JB) = (1.0-TRATIO)*TINNX(JB)+TRATIO*TINO(JB)
    DO JC=1,NACIN
      CIN(INCN(JC),JB) = (1.0-CRATIO)*CINNX(INCN(JC),JB)
                         +CRATIO*CINO(INCN(JC),JB)
    END DO
  END IF
END IF
```

The interpolation routines for other boundary condition data are similar. Note linear interpolation may not reproduce water-in-storage values used in volume balances to compute reservoir inflow rates.

Subroutine HEAT_EXCHANGE

This subroutine is used to compute the linearized surface heat exchange parameters - equilibrium temperature [ET] and coefficient of surface heat exchange [CSHE]. These terms are discussed fully in Appendix A, page A17-A21. Note these terms are required for the simplified ice computations as well as the equilibrium temperature approach to surface heat exchange.

Also required in either approach to computing surface heat exchange is the solar radiation rate. In this subroutine, it is computed from time, solar altitude and cloud cover (Ryan and Stolzenbach, 1972; Wunderlich, 1972).

Equilibrium temperature is computed iteratively using the methods in Edinger, et al. (1974). The calculations are done in British units and converted to SI units prior to the return.

Subroutine RADIATION

Subroutine RADIATION computes net solar radiation (incoming minus that reflected at the surface, usually 6%) and longwave atmospheric radiation (Wunderlich, 1972).

Subroutine SURFACE_TERMS

The two previously discussed subroutines compute surface heat exchange terms dependent only on the observed meteorological data and are called once for each timestep. These terms account for four of the seven terms involved in surface heat exchange: incident solar (shortwave) radiation, reflected shortwave radiation, and incoming atmospheric (longwave) radiation. The other three terms (back radiation from the water surface, evaporative heat flux and conductive heat flux) are dependent on the water surface temperature and need to be computed for each segment at each timestep. Note with the linear approximations to surface heat exchange (equilibrium temperature and the coefficient of surface heat exchange), the surface temperature dependent terms are approximated and this approach does not require reference to the water surface temperature. This feature was the prime reason for their use prior to generally available fast computers.

Subroutine PRINT_GRID

This subroutine is called under control of the snapshot logic (see Task 2.8). It prints snapshots over time of elevations, velocities, temperatures, and constitu-

ent concentrations. The coding is straightforward but several features are worth noting. First, the results are not directly written from their computational arrays (ie, [U]), but instead to a character variable [CONV]. The latter variable contains blanks in the locations representing inactive cells. This permits only active cell information to be displayed in the snapshot file - writing the variables directly to the snapshot file would show zeros at locations of inactive cells. Also note the logic for long and short forms. Logical variables are also used to control which arrays are output. These may be traced from the user specification of them on the **Constituent Output** card (see page C74).

Subroutine SELECTIVE_WITHDRAWAL

The selective withdrawal algorithm calculates the vertical limits of the withdrawal zone based on the boundary outflows, outlet geometry, and in-pool densities. The algorithm then assigns flows for each layer within the calculated withdrawal zone.

The subroutine is called for each branch (assuming the user has selected this computation) in Task 2.1. The main computational loop computes, for each structure in the branch, the upper and lower withdrawal limits in terms of the model's layer numbers. The velocity and flow associated with each structure are then computed. Once this loop is completed, the flows for all structures are combined. Boundary horizontal velocities [U] and outflows [QOUT] previously computed but are now beyond the range of the withdrawal limits are reset to zero.

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13. ABSTRACT (Maximum 200 words)

This manual describes and provides guidance for the use of CE-QUAL-W2 V2.0, a two-dimensional, longitudinal/vertical, hydrodynamic and water quality model. The model was originally developed by the Environmental and Hydraulics laboratories, U.S. Army Engineer Waterways Experiment Station, and is suitable for applications to rivers, lakes, reservoirs, and estuaries. Version 2.0 is a result of major code modifications that have improved the mathematical description of the prototype, computational efficiency, and utility of the model.

The manual is organized into three chapters and four appendixes. Chapter 1 consists of an introduction to the model and the user manual. Chapter 2 describes the model's major capabilities and limitations. Chapter 3 provides an overview of the steps involved in applying the model including data preparation and model application. The appendixes provide the user with the information necessary to understand the model details. Appendix A describes the theoretical, numerical, and computational basis for the hydrodynamic portion of the model. Appendix B describes the theoretical and computational basis for the water quality portion of the model. Appendix C describes the preparation of input files. Appendix D describes the algorithms used in the code. An index is included in Appendix E. References include a partial bibliography of CE-QUAL-W2 applications.

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