

USERS MANUAL FOR A BRANCHED
LAGRANGIAN TRANSPORT MODEL

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CONVERSION FACTORS

The Branched Lagrangian Transport Model is capable of receiving input in either English or Metric (International System) units, so both unit systems are used in this report. The following conversion factors may be used to convert the units of measurement in this report.

<u>Multiply inch-pound units</u>	<u>by</u>	<u>To obtain metric units</u>
inch (in)	0.02540	millimeter (mm)
feet (ft)	0.3048	meters (m)
mile (mi)	1.609	kilometers (km)
square feet (ft ²)	0.0929	square meters (m ²)
cubic feet (ft ³)	0.02832	cubic meters (m ³)
feet per second (ft/s)	0.3048	meters per second (m/s)
feet per hour (ft/hr)	0.3048	meters per hour (m/hr)
miles per hour (mi/h) (km/hr)	1.609	kilometers per hour
cubic feet per second (ft ³ /s)	0.02832	cubic meters per second (m ³ /s)
kilopascal (kpa)	10.00	millibars (mb)
inches of mercury (in Hg)	33.864	millibars (mb)
milligrams per day per foot (mg/day-ft)	3.2808	milligrams per day per meter (mg/day-m)
Langley	1.0000	calories per square centimeter

Temperature Conversion: $^{\circ}\text{F} = 1.8^{\circ}\text{C} + 32$
 $^{\circ}\text{C} = (^{\circ}\text{F} - 32)/1.8$

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ABSTRACT

A Lagrangian transport model for simulating the fate of water-quality constituents, such as temperature and dissolved oxygen, in networks of open channels with reversing flow is presented in this Users Manual. One-dimensional transport theory, algorithms used in the model, and application of the model including two examples are presented. Appendices discuss three plot programs for use with the model and the Time-Dependent Data System for managing input and output data.

INTRODUCTION

Predictions of the fate and movement of dissolved constituents in rivers and estuaries are needed to understand the nature and scope of many water-quality problems. The ability to make such predictions partially depends on the development of suitable numerical transport models. Fortunately, dissolved constituents are laterally well-mixed in many rivers and estuarine channels and, therefore, transport models that represent channels as one-dimensional entities are often adequate.

A one-dimensional water-quality model based on the Lagrangian reference frame was previously developed for use in single-channel upland streams (Jobson 1980, Schoellhamer and Jobson 1986a, 1986b). Because of the accuracy and stability of this model, it has been generalized for use in a network of open channels with one-dimensional flow. This new generalized model, called the Branched Lagrangian Transport Model (BLTM), may be useful in simulating transport of a conservative substance such as dye or reactions between water quality constituents in branched river systems, tidal canal systems, and deltaic channels. The purpose of this report is to provide a potential model user sufficient information on the BLTM to determine its suitability for a given problem and to provide a user the information needed to correctly apply the model.

The BLTM solves the convective-dispersion equation by using a Lagrangian reference frame in which the computational nodes move with the flow. The one-dimensional equations are solved for up to 10 constituents moving in as many as 30 branches connected at junctions. The unsteady flow hydraulics must be supplied to the model and the constituent concentrations are assumed to have no effect on the hydraulics. A flow model, such as the one presented by Schaffranek and others (1981), can be used to supply the hydraulic information to the model. The reaction kinetics of the constituents can be supplied by the user.

This users manual briefly describes one-dimensional transport theory, the BLTM, and the application of the model. A single constituent example and a multiconstituent example with the popular QUAL-II water-quality model reaction kinetics (Roesner and others, 1977a, 1977b) are provided.

ONE-DIMENSIONAL TRANSPORT THEORY

In the Lagrangian reference frame, the continuity of mass equation is

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial \xi} \left(D \frac{\partial C}{\partial \xi} \right) + S + \Phi + K (C - CR), \quad (1)$$

in which C is concentration, t is time, D is longitudinal dispersion coefficient, K is rate of production of the constituent, CR is the equilibrium concentration (that is, the concentration at which the internal production ceases), Φ is the rate of change in concentration due to tributary inflow, S is the rate of production of concentration, which is independent of the concentration (zero-order production rate), and ξ is the Lagrangian distance coordinate given by

$$\xi = x - x_0 - \int_{t_0}^t u dt', \quad (2)$$

in which x is the Eulerian (stationary) distance coordinate along the river, u is the cross-sectional mean stream velocity, and x is the location of the parcel at time t .

Equation 1 is similar to the conservation of mass equation written in the Eulerian reference frame (Schoellhamer and Jobson, 1986b) but it does not contain the convection term, and the definition of the longitudinal coordinate ξ is somewhat different. The Lagrangian reference frame is used in this model because it is numerically advantageous compared to Eulerian models (Jobson 1980, Thompson 1984).

Equation 1 is solved for each constituent modeled. It is convenient to number the constituents and then all equations can be represented by a single expression of the form

$$\frac{\partial C_l}{\partial t} = \frac{\partial}{\partial \xi} \left(D \frac{\partial C_l}{\partial \xi} \right) + S_l + \Phi_l + \sum_{n=1}^m K_{l,n} (C - CR_{l,n}), \quad (3)$$

in which C_l , S_l , and Φ_l are as defined in equation 1, except that they apply to the specific constituent l . The summation term allows for the interaction between constituents where $K_{l,n}$ is the rate coefficient for the production of constituent l due to the presence of constituent n , and $CR_{l,n}$ is the concentration of constituent n at which the production of constituent l due to n ceases.

Integration of equation 3 over the time interval Δt gives

$$C_l(t+\Delta t) = C_l(t) + \frac{\partial}{\partial \xi} \int_t^{t+\Delta t} D \frac{\partial C_l}{\partial \xi} dt + \int_t^{t+\Delta t} \Phi_l dt + \int_t^{t+\Delta t} [S_l + \sum_{n=1}^m K_{l,n} (C - CR_{l,n})] dt \quad (4)$$

Each term in equation 4 represents the contribution of a specific physical process to the change in concentration of the fluid parcel during the time interval Δt . An accumulation of each integral separately quantifies the contribution of each physical process to the concentration. A knowledge of the magnitude of each of these terms is very helpful in model calibration and data interpretation. The BLTM retains the value of each of the integrals in equation 4 except for the effect of tributary inflow.

Equations 1 through 4 apply only to a single fluid parcel and, therefore, do not give the variation of concentration in space and time directly. Parcels are assumed to be completely mixed, and their volume is changed only by tributary flows. The variation of concentration in a river reach is approximated by solving equation 1 for a series of parcels spaced along the river at intervals of about $u\Delta t$. The concentration at any point is the concentration of the parcel at that point.

The assumption of completely mixed parcels may cause interpolation errors when determining the concentration at a given point. The major reason for the accuracy of a Lagrangian model, in comparison to an Eulerian model, is that this interpolation error can occur only when output is desired and the resulting grid concentration is not used in further computations. In an Eulerian model, similar interpolation errors are made for every time step and grid point but the interpolated values are used as the basis of all further computations.

The solution scheme starts with a series of parcels in the river (the initial conditions) and adds a new parcel at each external boundary node with flow into the system during each time step (the boundary conditions). Equation 4 is numerically integrated for each parcel and for each constituent during each time step. The locations of the parcels are tracked by use of equation 2.

The advantages of a Lagrangian approach, as outlined above, are: (1) the scheme is very accurate in modeling the convection and dispersion terms in comparison to the usual Eulerian approach (Jobson 1980, Thompson 1984), (2), the Lagrangian model is stable for any time step (Jobson 1981), (3) the computer code for the algorithms is short, (4) the conceptual model directly represents the actual transport processes, (5) the model is economical to run, and (6) the model output includes helpful calibration and interpretation information that is not usually available from an Eulerian model.

THE BRANCHED LAGRANGIAN TRANSPORT MODEL

Figure 1 illustrates the example network used later in this report. Here, it will be used to demonstrate how the BLTM schematizes river systems. The system contains six branches connected by two interior junctions. Each branch must start and end at a junction.

The junctions must be numbered sequentially without skipping or repeating numbers. Interior junctions must be numbered first followed by exterior junctions. Modeling efforts will be made easier if these restrictions are considered when originally numbering a branch network for hydraulic modeling so that the same numbering system can be used for both hydraulic and subsequent transport modeling. A maximum of 29 internal junctions are allowed unless the program is redimensioned. Any number of branches may begin or end at a junction.

The branches are considered to be one dimensional river segments and can be numbered in any order as long as the numbering system starts with 1 and no numbers are skipped. A maximum of 30 branches are allowed unless the program is redimensioned. Each branch can be represented by up to 19 cross sections located at model grid points.

The grid points within each branch must be numbered sequentially starting at 1. A grid point must occur at each end of the branch. Numbering can start at either end but grid point number 1 is considered to be the upstream end of the branch in the program so positive discharge moves from grid point 1 to 2 to 3 The grid points do not have to be equally spaced and there is no restriction on the distance between grid points. The cross sectional area and top width in a reach between two adjacent grid points are equal to the average of the two grid point values, so as the grid spacing increases the resolution of spatial variability in flow is reduced. The initial number of parcels per reach is given by the user for every branch. A maximum of 26 parcels is allowed in each branch. If more than 24 parcels are in a branch at the end of a time step, the model combines the smallest parcel in the branch with the smallest of the two parcels adjoining it progressively until the number is reduced to 24. This allows room to add 2 parcels, one at each end of the branch, during the next time step. Initially no more than 24 parcels should be placed in any branch.

The transport model solves equation 4 for each constituent in each parcel in a branch during each time step. All the water to flow into either end of the branch is considered to constitute a new parcel and each parcel which flows out of the branch is mixed with all other water flowing into a junction before this water enters another branch.

Reactions or source rates which are location dependent (such as a reaction coefficient which is depth dependent) are determined for the entire parcel based on the reach averaged conditions in the reach occupied by the upstream boundary of the parcel. This occurs even though the parcel may physically span several reaches in the model. The rates are updated as the upstream parcel boundary passes each grid point. Parcels which pass out of a branch before the end of a time step experience reaction rates for the rest of the time step based on conditions in the last subreach of the branch. No reactions occur as the parcel enters a branch.

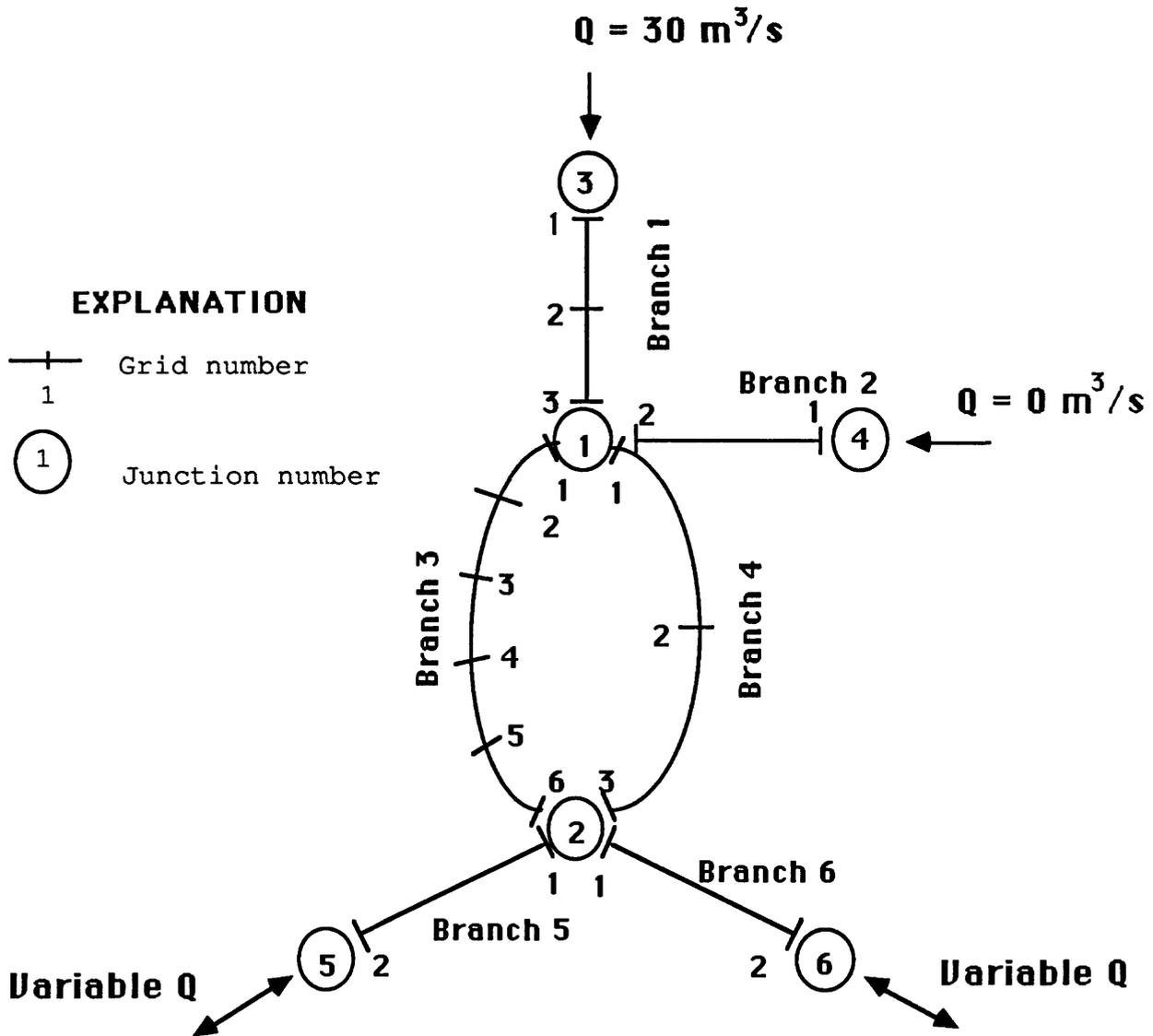


Figure 1.--Network for the example applications of the Branched Lagrangian Transport Model (BLTM).

Excessive use of interior junctions, may limit the ability of the model to accurately simulate dispersive fluxes. Dispersion occurs between parcels in a particular branch but not between branches. In other words, it is assumed that junctions represent points of zero dispersive flux. All mass passing through a junction, however, is mixed before entering the next branch so numerical dispersion may also occur at junctions.

For each time step the flow conditions must be supplied to the model from an external file. The four required hydraulic values at every grid point are discharge, cross-sectional area, top width, and tributary inflow. Top width is utilized only in the user-written decay coefficient subroutine, so an accurate value is needed only if top width is used in the subroutine. The tributary is assumed to exchange flow with the river just upstream of the grid point. The flow field can be supplied either in a sequential file as would usually be output by a user-supplied flow model or by the Time-Dependent Data System (TDDS) (Regan, written communication, 1986) supplied with the BRANCH flow model of Schaffranek and others (1981). If the TDDS is used, tributary inflow only needs to be supplied where it is nonzero.

As pointed out above, the model is dimensioned to allow a maximum of 10 constituents, 30 branches, 29 internal junctions, 19 grid points per branch, and 26 parcels per branch. These numbers were deliberately selected to be different and unique. If one wishes to redimension the model to allow a greater or lesser size of these arrays, it is necessary to edit the model and change all INTEGER and REAL statements which contain these numbers. It is also necessary to change the value of variables NOCO, NOBR, NOIJ, NOSC, or NOPR (for the maximum number of constituents, branches, internal junctions, cross sections, and parcels, respectively) which are assigned values immediately after the REAL statement in the main program.

The dispersion integral is evaluated by use of a simple, explicit finite difference approximation

$$\int_t^{t+\Delta t} \frac{\partial}{\partial \xi} (D \frac{\partial C}{\partial \xi}) dt = \frac{|Q|\Delta t}{PV} (D_f^+ (C^+ - C^-) - D_f^- (C - C^-)), \quad (5)$$

in which Q is the channel discharge, PV is the parcel volume, Δt is the time step, D_f^+ and D_f^- are dimensionless dispersion factors at the upstream and downstream ends of the water parcel, and C^+ and C^- are the concentrations in the parcels which are upstream and downstream of the parcel in question, respectively. All concentrations on the right hand side of equation 5 are evaluated at the previous time step.

The dimensionless dispersion factor D_f is defined as

$$D_f = \frac{D}{|u|\Delta x}, \quad (6)$$

in which Δx is the parcel length. D_f is the ratio of the interparcel mixing rate to the channel discharge and is equivalent to the inverse of the Peclet number. For steady flow $\Delta x = |u|\Delta t$, which allows estimation of D_f for steady flows given D and for unsteady flows given D and a representative u (Schoellhamer and Jobson, 1986a). For a large time step the value of D_f is small, the parcels are far apart, and equation 5 may underestimate the concentration gradients and dispersive fluxes. For small time steps the value of D_f is large and the parcels are very close together. Because equation 5

allows material to diffuse through only one parcel per time step, equation 5 does not spread the material fast enough for very small time steps. The BLTM eliminates this restriction and enforces stability by subdividing the dispersion time step on a parcel by parcel basis as described by Schoellhamer and Jobson (1986a).

Because the dispersive flux is proportional to the discharge, the simulated dispersion would normally be zero when the discharge is zero. The user can specify a minimum dispersive velocity in order to allow dispersion to continue at low discharges. The minimum interparcel mixing rate is one-half the product of cross-sectional area and minimum dispersive velocity. The specified minimum dispersive velocity should be representative of the water velocity caused by non-flow induced effects, such as wind.

More elaborate techniques to approximate dispersion, such as used by Thomson et al. (1984), have not been needed for any conditions encountered so far. These have included problems with very large concentration gradients (Jobson, 1980) and highly unsteady flows (Jobson, 1985).

Reaction kinetics vary greatly from problem to problem so the BLTM is designed to allow the user to supply these kinetics. The specific reaction kinetics are controlled by the values of S_t , $K_{t,n}$, and $CR_{t,n}$ in equation 4. These coefficients are normally set to zero, indicating a conservative constituent unless defined otherwise by a user-supplied decay-coefficient subroutine called FINK. The coefficients can be constants or variables and can be functions of location, local hydraulic variables, time, concentration of any of the constituents, or an externally supplied variable such as wind speed or solar radiation. Examples are given in the next section of a FINK for a single conservative constituent and a FINK which duplicates the reaction kinetics in the QUAL-II model by Roesner and others (1977a, 1977b). Another example of reaction kinetics for oxygen, BOD and the nitrogen cycle is given by Jobson (1985).

APPLICATION OF THE BRANCHED LAGRANGIAN TRANSPORT MODEL

Capabilities, Restrictions, and Availability

The BLTM can simulate the movement and fate of up to 10 water-quality constituents in a network of interconnected open channels with unsteady reversing flows. The restrictions of the model include one-dimensional channels, unstratified flow, and fixed channel geometry. The BLTM does not perform hydraulic computations. The flow field at fixed grid points, including discharge, cross-sectional area, and top width must be provided by the user. The user can define the constituents and the constituents's reaction kinetics by writing the necessary FORTRAN computer code in a subroutine. Preparation of this subroutine is not difficult and may be necessary depending upon the specific needs of the user.

All FORTRAN programs and input files mentioned in this report are available from the Office of Surface Water, U. S. Geological Survey, Mail-Stop 415, Reston, VA 22092. The following is a summary of the input and output files used or generated by the BLTM, and two example BLTM applications.

Input Files

BLTM.IN

The basic input file which is always needed is called BLTM.IN. It sets up the simulation, defines the program options to be used and defines the physical system being modeled. Figure 2 contains a copy of BLTM.IN used in the one constituent example. Appendix A contains a description of the input data for BLTM.IN. Unless specified otherwise, all input cards are set up to contain a 10 column field for the card label followed by 10 fields of 7 columns each. For left justification in the input fields, the card label should start in column 1 and the other fields should start in columns 11, 18, 25, 32, 39, 46, 53, 60, 67, and 74.

As can be seen from figure 2 and Appendix A, the first example problem will contain 6 branches, 2 interior junctions (see figure 1), and 24 time steps will be modeled. The second input card also indicates that 1 constituent will be simulated, the model starts at midnight (JTS = 0), the output will be printed every 6 time steps in both BLTM.OUT and PARCEL.OUT, the TDDS will be used for hydraulic and boundary condition data (ITDDS = 2) and the input units are in meters except for river miles (IENG = 0). The floating point header card indicates that the model will be run with a time step of 1.0 hour and the minimum dispersive velocity will be assumed to be 0.1 m/s. The constituent label card indicates that the name of constituent number 1 is DYE and the change in concentration due to the presence of constituent 1 will be tabulated as PDC in the output file BLTM.OUT. The branch information cards for the example indicate that branch 1 contains 3 grid points (see figure 1) and has a dispersion factor of 0.3. The card also indicates that branch 1 extends from junction 3 (an external junction because $3 > \text{NJNCT} = 2$) to junction 1 and initially there is one parcel per reach (IPPR = 1). Three additional cards are needed because the branch has 3 grid points and the simulation has less than nine constituents. Grid point 2, for example, is 0.303 miles downstream of the reference point, output is not desired in BLTM.OUT (IOUT = 0) and the initial concentration between grid points 2 and 3 is 1.0. Card 3 is not required because less than nine constituents are simulated.

Data sets 6 through 10 are only needed if the TDDS is used. Data set 6 indicates that 4 data types are input from the TDDS, no time series are output to the TDDS, and no TDDS summaries will be printed. Data set 7 indicates the simulation starts in 1986, month 5, day 22, hour 0, minute 00 and ends in 1986, month 5, day 22, hour 24, minute 00. Data set 8 contains the station identification numbers for each grid point read in starting with branch 1 which has station identification number of 00000011, 00000012, and 00000013 for grid points 1, 2, and 3, respectively. Data set 9 indicates that flow data (Q, A, and B) contain 96 readings per day (the flow model was operated with a 15 minute time step) which will be retrieved from the TDDS for every grid point by default. Input concentration (C1) contain 24 readings per day, with 4 grid points containing data (the 4 external boundaries) and the grid points are at branch 1 grid point 1, branch 2 grid point 1, branch 5 grid point 2, and branch 6 grid point 2.

```

EXAMPLE 1 FOR BLTM.F77 WITH SINGLE CONSERVATIVE CONSTITUENT
HEADER 1      6      2      24      1      0      6      6      0      0
HEADER 2      1.00    0.1
LABEL        1      DYE      1
BRANCH P 1    3      0.30    3      1      1
B 1 SC 1     0.000    0      1.0
B 1 SC 2     0.303    0      1.0
B 1 SC 3     0.606    0
BRANCH 2      2      0.30    4      1      1
B 2 SC 1     0.000    0      2.0
B 2 SC 2     1.420    0
BRANCH 3      6      0.30    1      2      1
B 3 SC 1     0.000    0      3.0
B 3 SC 2     0.472    0      3.0
B 3 SC 3     0.947    0      3.0
B 3 SC 4     1.420    1      3.0
B 3 SC 6     2.367    0
BRANCH 4      3      0.30    1      2      1
B 4 SC 1     0.000    0      4.0
B 4 SC 2     0.852    0      4.0
B 4 SC 3     1.705    0
BRANCH 5      2      0.30    2      5      1
B 5 SC 1     0.000    0      5.0
B 5 SC 2     1.042    0
BRANCH 6      2      0.30    2      6      1
B 6 SC 1     0.000    0      6.0
B 6 SC 2     1.042    1
TDDS CARD_4  0      0
TDDS DATE_86 5      22      0      00      86      5      22      24      00
TDDS STID_   00000011  00000012  00000013
TDDS STID_   00000021  00000022
TDDS STID_   00000031  00000032  00000033  00000034  00000035
TDDS STID_   00000036
TDDS STID_   00000041  00000042  00000043
TDDS STID_   00000051  00000052
TDDS STID_   00000061  00000062
TDDS INPT_   Q96
TDDS INPT_   A96
TDDS INPT_   B96
TDDS INPT_   C124      4      1      1      2      1      5      2
TDDS INPT_6  2

```

Figure 2.--Input data file BLTM.IN for the single constituent example using TDDS for flow and boundary conditions.

Boundary conditions are read from the TDDS and the concentration for the boundary or tributary inflows must represent the average concentration during the time step. For example the first boundary concentration at branch 1, grid point 1 should represent the average concentration of the inflow between time zero and Δt . Boundary condition values are required at all external junction for every time step. Of course, if the flow at the junction is zero or out of the system the numerical value of the concentration is immaterial. Boundary conditions can also be read from BLTM.IN if ITDDS is equal to 0 or 1. In this case, the number of boundary conditions that change during each time step (NBC) is read and the branch, grid point, and value of every changed boundary condition is read. All boundary conditions (external junctions and tributaries) are initially set to zero. For example, a constant zero boundary condition does not have to be specified and a constant nonzero boundary condition needs to be specified only for the first time step. These conditions will be illustrated in the second example application.

Flow Field

The flow field is read from either a time-dependent data base (TDDB) with the TDDS or a sequential file called BLTM.FLW. The TDDS also requires a data station reference file which contains identification numbers of all the grid points (Regan, written communication, 1986). The first 36 lines of the sequential file BLTM.FLW used in the QUAL-II example are shown in figure 3. The first 15 columns are ignored by the BLTM but are used to record the time step and branch and grid point numbers so that the user can easily identify hydraulic data at a specific grid point and time step. Each line contains the discharge, area, top width, and tributary inflow for the time step indicated in the first five columns, the branch indicated in columns six thru ten, and the grid point indicated in columns 11 thru 15. The format of each line is 3I5,4E18.5. All values in BLTM.FLW are the average values during the time step at the grid point. All values in the TDDB, however, are instantaneous values at the grid point.

FINK.IN

Another input file (FINK.IN) is opened and read from subroutine FINK. Because the user is expected to modify this subroutine to suit the particular needs of the problem, the input format for this file is quite flexible. In general this file is to be used to input constant coefficients used to define the reaction kinetics and time varying information, such as wind speed, air temperature, or solar radiation, used in computing the reaction rates. The first example considers a single conservative constituent so all coefficients normally set up in subroutine FINK are zero. Since the decay coefficients are set to zero before FINK is called, FINK does nothing and no input file is required in this case. A listing of the subroutine FINK used in example the single constituent is shown in figure 4. Notice that the coding which would normally open the input file and read input data is commented out. This input will be discussed in more detail when the second example is discussed.

1	1	1	0.30000E+02	0.35652E+03	0.16404E+03	0.00000E+00
1	1	2	0.28185E+02	0.35637E+03	0.16404E+03	0.00000E+00
1	1	3	0.26310E+02	0.35630E+03	0.16404E+03	0.00000E+00
1	2	1	0.00000E+00	0.13011E+03	0.60000E+02	0.00000E+00
1	2	2	-0.33050E+01	0.13032E+03	0.60000E+02	0.00000E+00
1	3	1	0.17480E+02	0.20686E+03	0.95240E+02	0.00000E+00
1	3	2	0.15330E+02	0.22697E+03	0.10474E+03	0.00000E+00
1	3	3	0.12295E+02	0.24728E+03	0.11429E+03	0.00000E+00
1	3	4	0.87100E+01	0.26810E+03	0.12381E+03	0.00000E+00
1	3	5	0.55300E+01	0.28873E+03	0.13333E+03	0.00000E+00
1	3	6	0.19450E+01	0.30936E+03	0.14286E+03	0.00000E+00
1	4	1	0.55800E+01	0.78195E+02	0.36000E+02	0.00000E+00
1	4	2	0.45000E+01	0.77915E+02	0.36000E+02	0.00000E+00
1	4	3	0.29800E+01	0.77960E+02	0.36000E+02	0.00000E+00
1	5	1	0.12020E+02	0.10827E+02	0.50000E+02	0.00000E+00
1	5	2	0.71350E+01	0.10625E+02	0.50000E+02	0.00000E+00
1	6	1	-0.71050E+01	0.12632E+02	0.58330E+02	0.00000E+00
1	6	2	-0.12645E+02	0.12921E+02	0.58330E+02	0.00000E+00
2	1	1	0.30000E+02	0.36324E+03	0.16404E+03	0.00000E+00
2	1	2	0.26400E+02	0.36294E+03	0.16404E+03	0.00000E+00
2	1	3	0.22700E+02	0.36277E+03	0.16404E+03	0.00000E+00
2	2	1	0.00000E+00	0.13249E+03	0.60000E+02	0.00000E+00
2	2	2	-0.64300E+01	0.13269E+03	0.60000E+02	0.00000E+00
2	3	1	0.12925E+02	0.21062E+03	0.95240E+02	0.00000E+00
2	3	2	0.90600E+01	0.23150E+03	0.10474E+03	0.00000E+00
2	3	3	0.43700E+01	0.25278E+03	0.11429E+03	0.00000E+00
2	3	4	-0.64500E+00	0.27411E+03	0.12381E+03	0.00000E+00
2	3	5	0.48800E+01	0.29532E+03	0.13333E+03	0.00000E+00
2	3	6	0.90600E+01	0.31661E+03	0.14286E+03	0.00000E+00
2	4	1	0.33550E+01	0.79615E+02	0.36000E+02	0.00000E+00
2	4	2	0.13550E+01	0.79730E+02	0.36000E+02	0.00000E+00
2	4	3	-0.61000E+00	0.79785E+02	0.36000E+02	0.00000E+00
2	5	1	0.55700E+01	0.11081E+03	0.50000E+02	0.00000E+00
2	5	2	0.49000E+00	0.11050E+03	0.50000E+02	0.00000E+00
2	6	1	-0.15260E+02	0.12928E+03	0.58330E+02	0.00000E+00
2	6	2	-0.21495E+02	0.13388E+03	0.58330E+02	0.00000E+00

Figure 3.--Sample hydraulic input file BLTM.FLW for QUAL-II example (first two time steps shown).

Output Files

The output of the BLTM is stored in two files, BLTM.OUT and PARCEL.OUT. BLTM.OUT is designed to provide information to the modeler directly and PARCEL.OUT stores information which can be used by post-processor programs such as the plot programs in Appendices A and B.

Figure 5 contains BLTM.OUT for the one constituent example. BLTM.OUT echos input information from BLTM.IN and presents the results in a readable form. It also prints the simulation results at selected grid points and at a selected time interval. The results contain the time, branch number, grid point number, parcel number located at the grid point, the volume of the parcel (PV), the volume of the portion of the parcel which is upstream of the grid point (VU), and the time that the parcel entered the branch (PH). For each constituent the output lists the current concentration of the parcel, the concentration the parcel had when it entered the branch (PTI), the change in concentration which has occurred in the branch because of dispersion (PDF) and the change in concentration which has occurred in the branch because of reaction with constituent LR(L) (PDC). The array PDC is the integral over time since the parcel entered the branch of the term LR(L) of the summation shown in equation 4. The expression for PDC is

$$PDC(t) = \int_{t_e}^t K_{l,n} (C_n - CR_{l,n}) dt, \quad (7)$$

in which $n = LR(L)$ and t_e is the time the parcel entered the branch.

The second output file PARCEL.OUT contains the location and concentration of all parcels in the system at specified time intervals. This file is intended to be used with post-processor programs to present the results in any number of ways because, if the output time interval is set to 1, the file contains a complete record of the space time variation of concentrations as computed by the model. Appendix C describes a program to plot the concentration of any constituent as a function of time for any location in the system. Appendix D contains a plot program which will plot an instantaneous concentration profile of any of the constituents for one or a specified combination of branches. Both plot programs use data stored in PARCEL.OUT. Because PARCEL.OUT is used as an input file and it may be very lengthy, the user should review BLTM.OUT to determine the simulation results. The data stored in PARCEL.OUT will now be described in detail for the user with post-processing needs.

```

SUBROUTINE FINK (K,MX,J,NEQ,PV,PT,
$ Q,A,W,XK,S,CR,IRC,NNN,LUOUT)
C
C*** BEGIN DIMENSIONING DEFINITION
C
C NOBR      Maximum number of branches allowed in model
C NOPR      Maximum number of parcels allowed in branch
C           (NOPR should be at least 20 + 2 times NOCO)
C NOCO      Maximum number of constituents allowed
C
C
C INTEGER NOBR,NOPR,NOCO
C PARAMETER (NOBR=30, NOPR=26, NOCO=10)
C
C + + + LOCAL VARIABLES + + +
C INTEGER I,LUOUT
C REAL      XK(NOCO,NOCO),S(NOCO),CR(NOCO,NOCO),PT(NOCO,NOPR),
#          AK(NOCO,NOCO)
C COMMON NXSEC(NOBR),NBRCH,IENG
C SAVE      AK
C IF(IRC.NE.1)GO TO 2
C IF(J.NE.1)GO TO 2
C   WRITE(*,*)'Enter all decay coefficients in per hour'
C   DO 1 L=1,NEQ
C     WRITE(*,*)'Enter decay coefficient for constituent',L,' - '
C     READ(*,*)AK(L,L)
1 CONTINUE
2 CONTINUE
C   DO 3 L=1,NEQ
C     XK(L,L)=-AK(L,L)
3 CONTINUE
C   IRC=0
C   RETURN
C   END

```

Figure 4.--Listing of subroutine FINK for the transport of conservative substances.

THE 6 BRANCH MODEL HAS 2 INTERNAL JUNCTIONS IS RUN 24 TIME STEPS EACH 1.00 HOURS LONG.
 THE MODEL STARTS AT 0.00 HOURS PAST MIDNIGHT.
 THE GRID OUTPUT IS GIVEN IN BLTM.OUT EVERY 6 TIME STEPS.
 THE PARCEL OUTPUT IS GIVEN IN PARCEL.OUT EVERY 6 TIME STEPS.
 1 CONSTITUENTS ARE ROUTED AND THE MINIMUM DISPERSIVE VELOCITY IS 0.100 M/S.
 BOUNDARY CONDITIONS READ FROM TDDB
 FLOW FIELD READ FROM TDDB
 INPUT UNITS ARE METRIC (METERS) EXCEPT RIVER MILES

INITIAL CONDITIONS

GRID	RIVER MILE	DISCHARGE CU M/S	AREA SQ M	TOP WIDTH METERS	TRIB. FLOW CU M/S	DYE	INITIAL CONCENTRATION
BRANCH 1 DQQ= 0.30 EXTENDS FROM JUCT 3 TO JUNCTION 1							
1	0.00	30.00	356.32	164.04	0.00	1.00	
2	0.30	28.18	356.37	164.04	0.00	1.00	
3	0.61	28.31	356.30	164.04	0.00		
BRANCH 2 DQQ= 0.30 EXTENDS FROM JUCT 4 TO JUNCTION 1							
1	0.00	0.00	130.11	60.00	0.00	2.00	
2	1.42	-3.31	130.12	60.00	0.00		
BRANCH 3 DQQ= 0.30 EXTENDS FROM JUCT 1 TO JUNCTION 2							
1	0.00	18.00	17.48	206.86	0.00	3.00	
2	0.47	30.00	15.33	226.97	0.00	3.00	
3	0.95	18.00	12.29	247.28	0.00	3.00	
4	1.42	18.00	8.71	268.10	0.00	3.00	
5	1.89	18.00	5.53	288.73	0.00	3.00	
6	2.37	18.00	1.94	309.36	0.00		
BRANCH 4 DQQ= 0.30 EXTENDS FROM JUCT 1 TO JUNCTION 2							
1	0.00	5.58	78.19	36.00	0.00	4.00	
2	0.85	4.50	77.91	36.00	0.00	4.00	
3	1.71	2.98	77.96	36.00	0.00		
BRANCH 5 DQQ= 0.30 EXTENDS FROM JUCT 2 TO JUNCTION 5							
1	0.00	12.02	108.27	50.00	0.00	5.00	
2	1.04	7.13	106.25	50.00	0.00		
BRANCH 6 DQQ= 0.30 EXTENDS FROM JUCT 2 TO JUNCTION 6							
1	0.00	-7.11	126.32	58.33	0.00	6.00	
2	1.04	-12.65	129.21	58.33	0.00		
DAY 1	HOUR 6.0	VU	PV	PH	DYE		
BR 3	GRID 4	K=10	0.200E+05	0.212E+06	-4.00	3.268	
				PTI		3.000	
				PDF		0.268	
				PDC		0.000	

Figure 5.--Sample of output file BLTM.OUT for single constituent example. (Continued on next page.)

BR	6	GRID	2	K= 5	0.360E+05	0.360E+05	6.00	10.000
								PTI
								10.000
								PDF
								0.000
								PDC
								0.000
DAY	1	HOUR	12.0		VU	PV	PH	DYE
BR	3	GRID	4	K=13	0.486E+05	0.165E+06	-1.00	2.423
								PTI
								3.000
								PDF
								-0.577
								PDC
								0.000
BR	6	GRID	2	K= 3	0.518E+05	0.518E+05	10.00	4.434
								PTI
								3.937
								PDF
								0.497
								PDC
								0.000
DAY	1	HOUR	18.0		VU	PV	PH	DYE
BR	3	GRID	4	K= 7	0.297E+05	0.934E+05	12.00	0.140
								PTI
								0.082
								PDF
								0.059
								PDC
								0.000
BR	6	GRID	2	K= 2	0.780E+05	0.780E+05	17.00	1.616
								PTI
								1.497
								PDF
								0.119
								PDC
								0.000
DAY	2	HOUR	0.0		VU	PV	PH	DYE
BR	3	GRID	4	K= 7	0.215E+05	0.996E+05	18.00	0.140
								PTI
								0.150
								PDF
								-0.010
								PDC
								0.000
BR	6	GRID	2	K= 6	0.770E+04	0.770E+04	24.00	10.000
								PTI
								10.000
								PDF
								0.000
								PDC
								0.000

Figure 5.-- Sample of output file BLTM.OUT for single constituent example (continued).

Figure 6 shows the first few lines of the file PARCEL.OUT for the single example constituent. The first line of data in figure 6 shows, for example, that at time step zero (the initial condition) branch 1 contained 2 parcels. The second line of the figure indicates that the upstream boundaries of these parcels relative to the grid schemitization were at 1.00 and 2.00 respectively. The third line indicates that the concentration of both parcels were 1.00. Similar initial condition data is repeated for the other five branches. Data were written to PARCEL.OUT only every 6 time steps so line 19 of the figure indicates that, at time step 6, branch 1 contained 5 parcels. The next line indicates the location of the upstream boundaries of each parcel expressed in grid units. For example parcel 2 located at 1.42 means that the upstream boundary of parcel 2 was located 42 percent of the way from grid point 1 to grid point 2. If more than one constituent had been modeled, the concentrations of constituent 2 would be given on a line after the concentrations of constituent 1. Branch 3 contains 16 parcels at time step 6. Twelve locations are printed on the first line and the remaining four are printed on the second line before giving the concentration.

Other output options included the plot program listed in Appendix E that plots any of the flow variables, as obtained from BLTM.FLW, for any branch and grid point as a function of time. Appendix F contains instructions for using the TDDS which can store BLTM output and write or plot any data set in the TDDB.

Conservative Transport Example

The first example of the model application will route a single conservative substance through the network illustrated in figure 1. The first step is to run a flow model to generate the hydraulic input to the transport model. For this example the hydraulic data were generated by use of a flow model documented by Schaffranek and others (1981) and using the TDDS to store the output results. All channels were assumed to be rectangular in shape and the bottom was assumed to be horizontal with an elevation of 9.61 meters. Other hydraulic data are shown in table 1. The discharges into branches 1 and 2 from the exterior junctions were assumed constant at 30.0 and 0.0 cubic meters per second respectively. The water surface elevations at the exterior junctions of branches 5 and 6 were assumed to be given by

$$Y = 11.778 + 0.3 \sin(2\pi(t - t_1)/24), \quad (8)$$

in which Y is the water surface elevation in meters, t is the time in hours, and t_1 is the lag time in hours. The value of t_1 was assumed to be 1.0 and 0.0 hours for branches 5 and 6, respectively. Figure 7 contains a plot of the variation of discharge with time at seven locations in the example problem. Negative and positive discharges occur in all branches except branch 1. The bulk of the flow moves down branch 3 rather than 4 and no net flow occurs in branch 2.

With the hydraulic data generated the transport model can be run. Figure 2 is a listing of the file BLTM.IN which is used for this example. The initial concentrations are assumed uniform in each branch with a value equal to the magnitude of the branch number. For example, branch 3 has an initial concentration of 3.0. The boundary concentrations during the simulation are read with the TDDS and they are assumed to remain constant at 0.0 for the upstream ends of branches 1 and 2 and 8.0 and 10.0 at the downstream ends of branches 5 and 6. No tributary inflow is assumed to occur.

```

0      1      2
1.00  2.00
1.00  1.00
0      2      1
1.00
2.00
0      3      5
1.00  2.00  3.00  4.00  5.00
3.00  3.00  3.00  3.00  3.00
0      4      2
1.00  2.00
4.00  4.00
0      5      1
1.00
5.00
0      6      1
1.00
6.00
6      1      5
1.00  1.42  1.83  2.25  2.67
0.00  0.04  0.08  0.15  0.22
6      2      7
1.00  1.67  1.69  1.75  1.81  1.88  1.95
1.86  1.58  1.29  1.02  0.76  0.61  0.25
6      3      16
1.00  1.18  1.33  1.46  1.61  1.80  2.05  2.64  3.28  3.93  4.61  5.30
5.40  5.57  5.78  5.94
0.25  0.79  0.97  1.27  1.64  2.04  2.45  2.76  2.98  3.27  3.77  4.53
5.33  6.09  6.54  9.30
6      4      13
1.00  1.09  1.13  1.17  1.22  1.30  1.43  2.11  2.73  2.74  2.82  2.92
3.00
0.25  1.40  1.62  1.97  2.42  2.94  3.50  4.12  4.81  5.51  6.15  6.51
9.30
6      5      7
1.00  1.02  1.09  1.64  1.73  1.87  1.98
9.30  5.48  5.59  6.41  7.17  7.56  8.00
6      6
1.00  1.17  1.43  1.68  1.89
9.30  9.61  9.89  9.98 10.00

```

Figure 6.--Sample of output file PARCEL.OUT for single constituent example.

Table 1.--Hydraulic variables for example problems

Branch	Grid	Distance (meters)	Width (meters)	Mannings n	Initial discharge (cu m/s)	Initial surface elevation (meters)
1	1		164.04	0.025	30.0	11.77
		1600.0				
	2		164.04	0.025	28.2	11.77
		1600.0				
	3		164.04	0.025	26.3	11.77
2	1		60.00	0.025	0.0	11.77
		7500.0				
	2		60.00	0.025	-3.3	11.77
3	1		95.24	0.0374	17.5	11.77
		2500.0				
	2		104.74	0.0374	15.3	11.76
		2500.0				
	3		114.29	0.0374	12.3	11.75
		2500.0				
	4		123.81	0.0374	8.7	11.75
		2500.0				
	5		133.33	0.0374	5.5	11.75
		2500.0				
	6		142.86	0.0374	1.9	11.75

Figure 8 contains a plot of the concentration profiles down each side of the network at six hour intervals. The initial concentrations are shown at time zero. Branch 1 is almost completely flushed after only six hours but the inflow at the lower ends of branches 5 thru 6 has increased the concentration in these branches. The inflow did not completely flush the initial water out of branch 5 and dispersion has increased the minimum concentration in branch 5 to 5.48 (Figure 6). The peak concentration in the lower end of branch 3 is water which entered the lower end of branch 6 with a concentration of 10.0 (the external boundary condition). Figure 7 illustrates that a much larger volume of water entered the lower end of branch 6 than entered the lower end of branch 5. Branch 6 contains all high concentration water which entered its lower end and this water has traveled up branches 3 and 4 a short distance. Low concentration water has entered branch 2 and moved upstream a short distance.

During the time from 6 to 12 hours positive flow (top to bottom in figure 1) exists almost everywhere. The downward displacement of the front is clearly evident in both branches 3 and 4. The concentration in branches 5 and 6 are reduced as the water is replaced by low concentration water from branches 3 and 4. The front in branch 2 moves only slightly downstream because the discharge at the lower end of the branch averages nearly zero during this 6 hour period. The plateau concentration in branch 2 (which is the parcel that originated in the branch) has reduced in concentration slightly (to 1.73 from 2.0) due to dispersive mixing with the low concentration water near the downstream end.

From 12 to 18 hours the maximum positive discharges occur in all branches. Most of the high concentration water has been flushed out of branches 3 and 4 and the concentration in branches 5 and 6 are much reduced. Branch 2 still has not displaced all of the low concentration water which entered the branch during the first eight hours of negative flow. Dispersion has reduced the branch 2 plateau concentration only slightly because dispersion does not occur past junctions and there was little low concentration water at the downstream end of the branch to mix with.

During the final six hours of the simulation all discharges are falling toward zero but all flows except at the downstream end of branches 2 and 6 remain positive. The concentration at the extreme lower end of branch 6 is 10.0 as would be expected since the flow there has reversed (Figure 7).

Individual profiles like those shown in figure 8 can be plotted by use of the program CXPLT.F77 described in Appendix D. The program uses data stored in PARCEL.OUT.

The concentration at the lower end of branch 2 is plotted as a function of time in figure 9. Concentration time plots like that shown in figure 9 can be plotted for any location in the system by use of the program CTPLT.F77 described in Appendix C. As can be seen in figure 9, the concentration at the lower end of branch 2 immediately falls from the initial value of 2.0 to 1.0 because the flow is into branches 2, and 3, from branch 1. During the next 7 hours the concentration falls and is always equal to the concentration of the water leaving branch 1. The flow reversal occurs between hour 8 and 9 so the concentration increases as the low concentration water exits the branch. The flow reversal occurs again between hours 23 and 24 so at 24 hours the concentration at the lower end of branch 2 becomes zero as the clear water from branch 1 starts to return to branch 2.

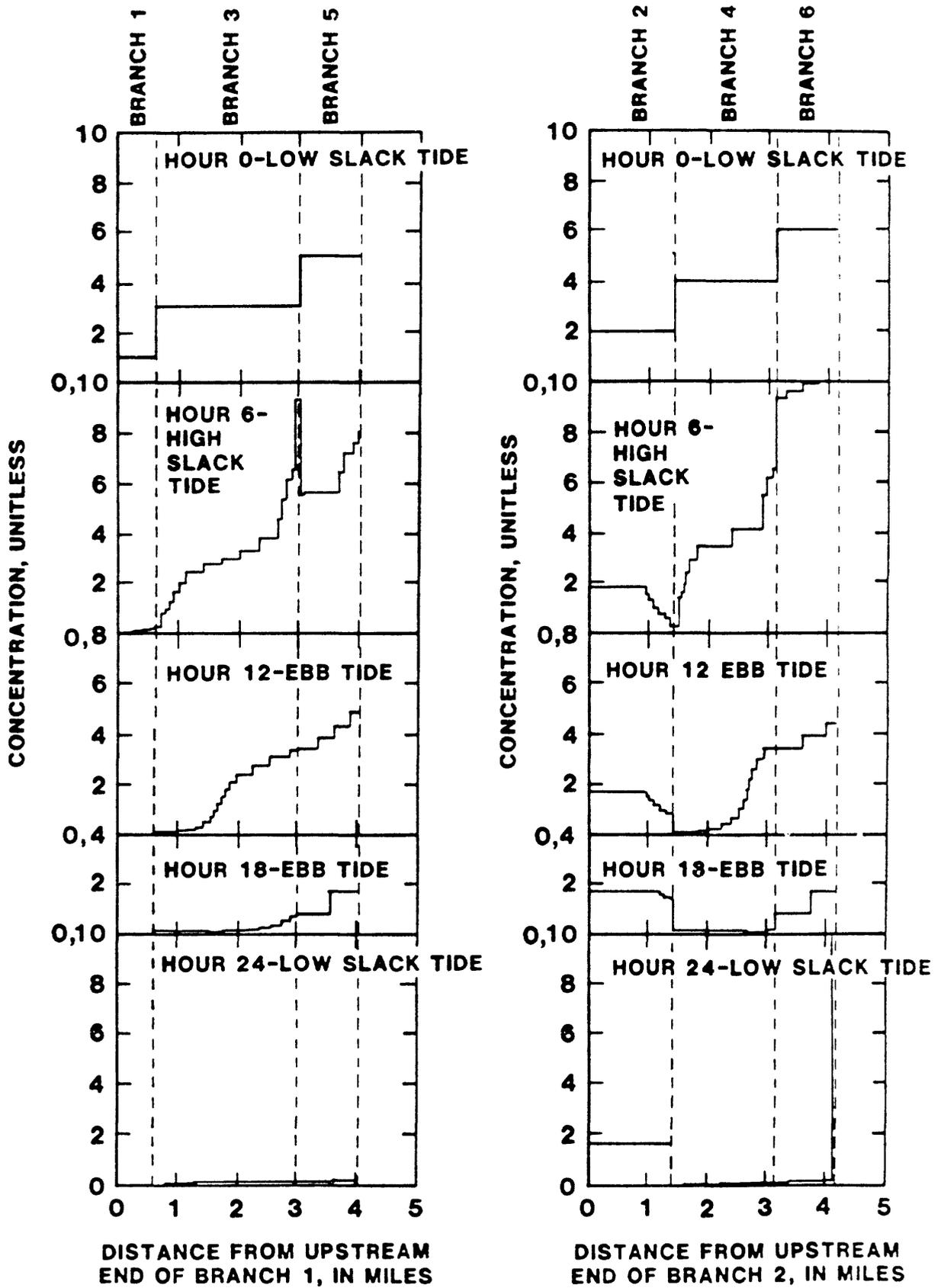


Figure 8.--Concentration profiles of a conservative substance in the example network at 6 hour intervals.

Table 1.--Hydraulic variables for example problems (Continued)

Branch	Grid	Distance (meters)	Width (meters)	Mannings n	Initial discharge (cu m/s)	Initial surface elevation (meters)
4	1		36.0	0.035	5.6	11.77
		4500.0				
	2		36.0	0.035	4.5	11.75
		4500.0				
	3		36.0	0.035	3.0	11.75
5	1		50.0	0.045	12.0	11.75
		5500.0				
	2		50.0	0.045	7.1	11.70
6	1		58.33	0.045	-7.1	11.75
		5500.0				
	2		58.33	0.045	-12.7	11.78

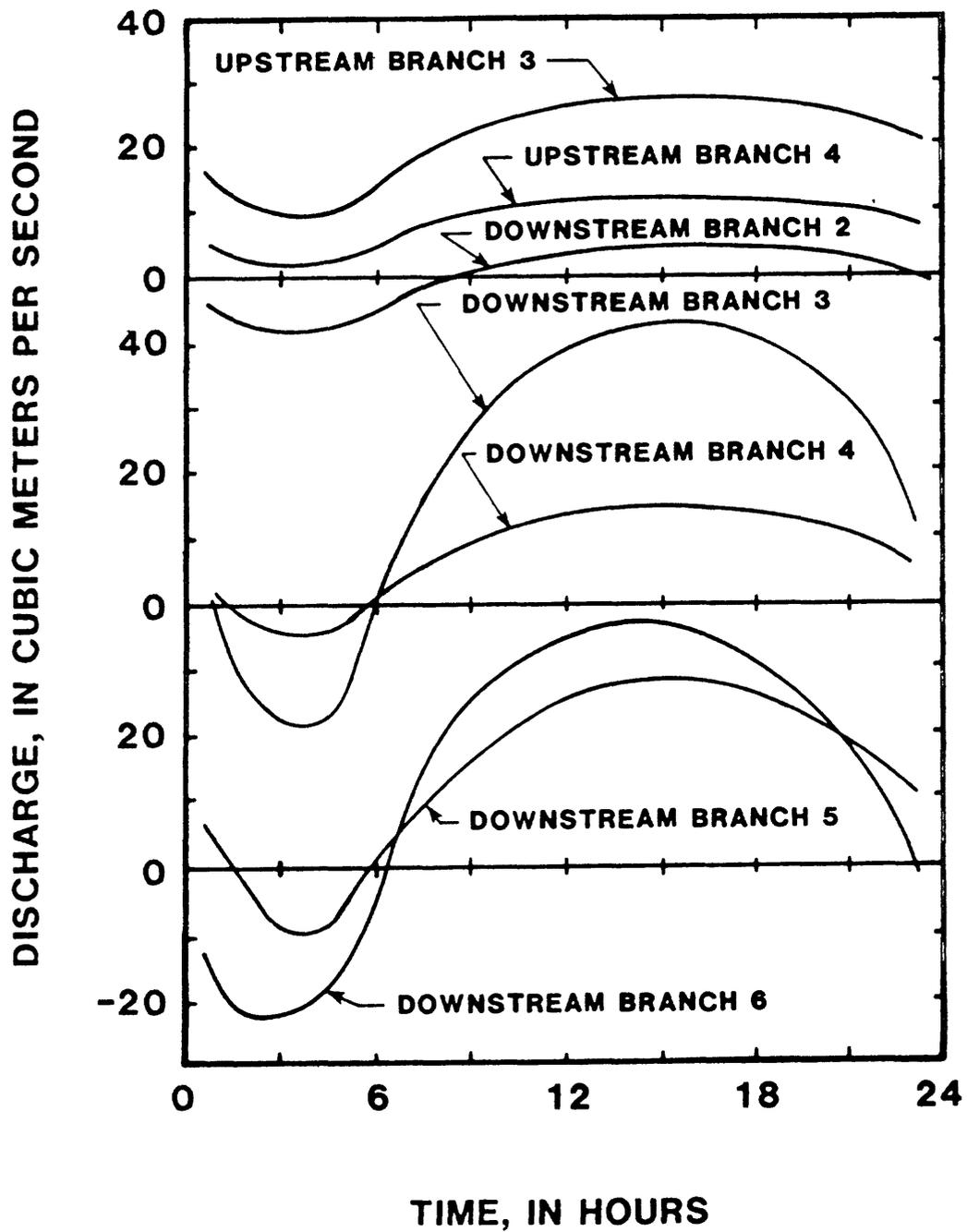


Figure 7.--Selected hydrographs for the example problems.

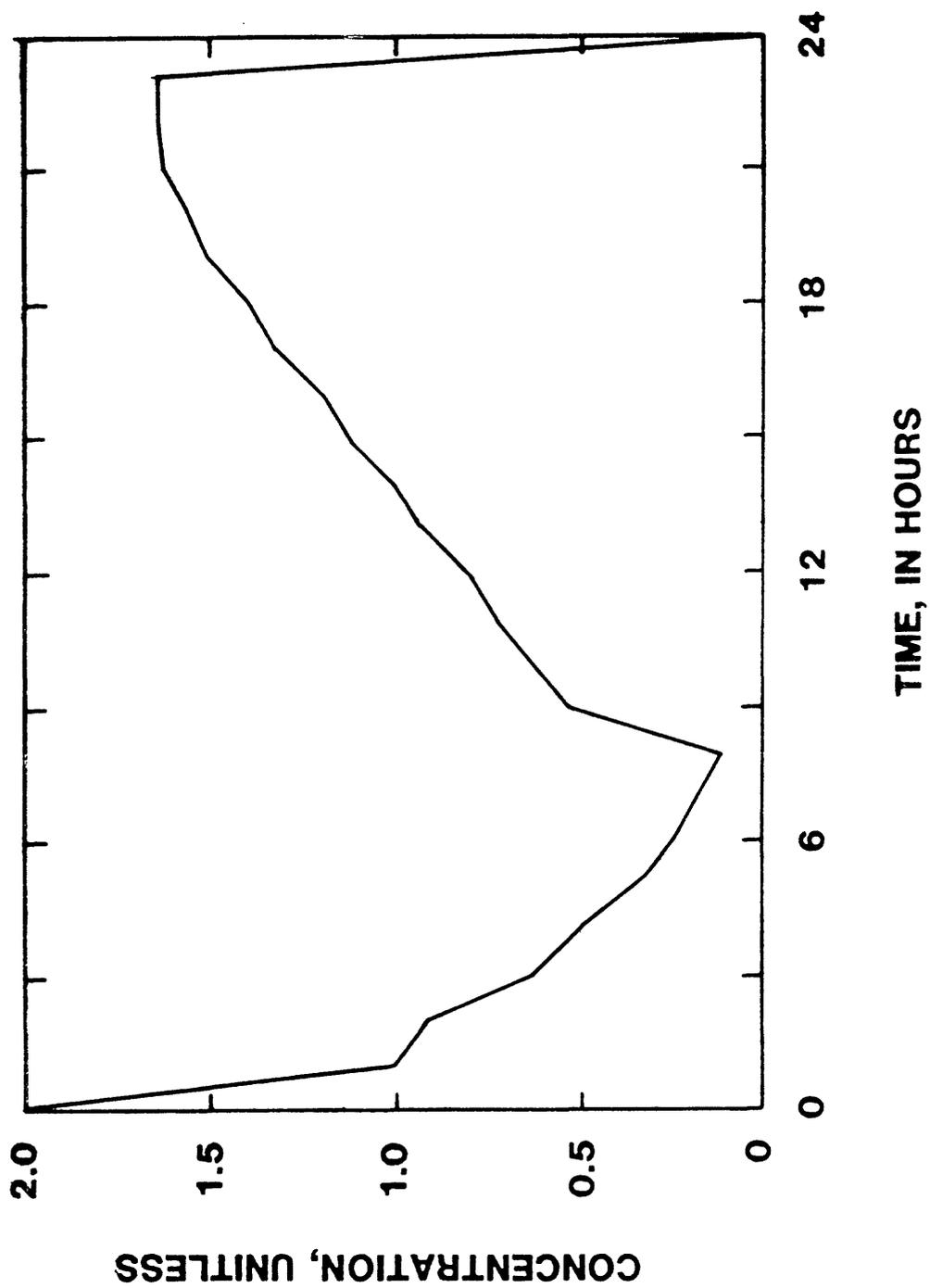


Figure 9.--Concentration at downstream end of branch 2, conservative example.

Figure 5 contains part of the output contained in BLTM.OUT for the example run. The first section of output is self-explanatory information which lists input data contained in BLTM.IN. Concentrations at two grid points (branch 3, grid point 4 and branch 6, grid point 2) are listed every 6 hours. After 6 hours, for example, the output indicates that the water parcel at grid point 4 in branch 3 had a volume (PV) equal to $2.12 \times 10^4 \text{ m}^3$ of which $2.00 \times 10^5 \text{ m}^3$ were upstream of the grid point (VU). This water was the tenth parcel downstream of the designated upstream end of the branch ($K = 10$) and the water entered the system at $\text{PH} = -4$. A negative entrance time indicates the water was in the system at time zero and the 4 indicates that the parcel was the fourth parcel from the upstream boundary at time zero. The concentration of the parcel of water was 3.268 and its concentration upon entering the system was $\text{PTI} = 3.0$ (the initial conditions). Dispersion has increased the concentration of this parcel by 0.268 because $\text{PDF} = 0.268$. Reactions have had no effect on the concentration of the parcel ($\text{PDC} = 0.0$) and there are no tributaries so its final concentration is its initial concentrations plus the change due to dispersion.

QUAL-II Example

The second example of the model will apply the QUAL-II reaction kinetics to the same flow field as that used in the first example. For the purposes of this example it will be assumed that a user-supplied flow model was used and the results were stored in the sequential file BLTM.FLW. Figure 3 contains a copy of the first 36 lines (2 time steps) of the file BLTM.FLW. Note that the data in figure 3 has been averaged over the time step while the TDDS data is composed of instantaneous values.

Figure 10 is a listing of the file BLTM.IN for this example. The second line of the file shows that 6 branches with 2 interior junctions are modeled for 24 time steps. Ten constituents are to be modeled, the model starts at midnight and output is printed every 6 time steps both in BLTM.OUT and PARCEL.OUT. In this example the TDDS is not used so $\text{ITDDS} = 0$ and the units are metric ($\text{IENG} = 0$). The second header card is identical to that used in the single constituent example. In this example ten label cards are needed, the first indicating that constituent 1 is called TEMP for temperature and the variable PDC will accumulate the temperature change that results from the presence of constituent 1 (surface heat exchange). Constituent 8 is called OXYG (oxygen) and the variable PDC will represent the change in oxygen concentration resulting from the presence of algae (constituent 2) in the branch. In other words, PDC for oxygen is the production of oxygen by algae since the parcel entered the branch. The branch definition cards are identical to those used in the first example except that initial conditions for ten constituents instead of one constituent must be defined for each reach. Note that all initial conditions are assumed uniform throughout the network and numerically equal to the constituent number except for temperature which is assumed to have an initial value of 10°C . No TDDS cards are necessary because the TDDS is not used but the boundary conditions of each constituent at each boundary must be defined.

For the first time step the boundary conditions will be specified at 4 locations (the four exterior junctions). The next four cards list the branch, grid point, and corresponding boundary values for the ten constituents. For all subsequent time steps the boundary conditions do not change so $\text{NBC} = 0$ for the remainder of the simulation. For example, the inflow temperatures at the external junctions to branches 1, 2, 5, and 6 are assumed constant at 25, 0, 15, and 15°C , respectively. If the flow is zero or out of the system at a boundary or tributary, no constituent mass is being added to the system so the boundary concentrations at that location are ignored for that time step.

EXAMPLE 2 FOR BLTM WITH QUALII KINETICS

HEADER 1	6	2	24	10	0	6	6	0	0		
HEADER 2	1.00	0.10									
LABEL	1	TEMP	1								
LABEL	2	ALGE	2								
LABEL	3	NH3	3								
LABEL	4	NO2	4								
LABEL	5	NO3	2								
LABEL	6	PHOS	2								
LABEL	7	BOD	7								
LABEL	8	OXYG	2								
LABEL	9	COLI	9								
LABEL	10	ARB	10								
BRANCH	1	3	0.30	3	1	1					
GRID	1	0.000	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	2	0.303	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	3	0.606	0								
BRANCH	2	2	0.30	4	1	1					
GRID	1	0.000	1	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	2	1.420	0								
BRANCH	3	6	0.30	1	2	1					
GRID	1	0.000	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	2	0.473	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	3	0.947	1	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	4	1.420	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	5	1.894	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	6	2.367	0								
BRANCH	4	3	0.30	1	2	1					
GRID	1	0.000	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	2	0.852	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	3	1.705	0								
BRANCH	5	2	0.30	2	5	1					
GRID	1	0.000	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	2	1.042	0								
BRANCH	6	2	0.30	2	6	1					
GRID	1	0.000	0	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
		9.00	10.00								
GRID	2	1.042	0								
TIME	1	4									

Figure 10.--Input file BLTM.IN for the QUAL-II example
(Continued on next page.)

BR	1SEC	1	25.00	2.00	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
BR	2SEC	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
BR	5SEC	2	15.00	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
BR	6SEC	2	15.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
TIME		2	0									
TIME		3	0									
TIME		4	0									
TIME		5	0									
TIME		6	0									
TIME		7	0									
TIME		8	0									
TIME		9	0									
TIME		10	0									
TIME		11	0									
TIME		12	0									
TIME		13	0									
TIME		14	0									
TIME		15	0									
TIME		16	0									
TIME		17	0									
TIME		18	0									
TIME		19	0									
TIME		20	0									
TIME		21	0									
TIME		22	0									
TIME		23	0									
TIME		24	0									

Figure 10.--Input file BLTM.IN for the QUAL-II example (Continued.)

This example uses the reaction kinetics of the popular QUAL-II water quality model (Roesner and others, 1977a, 1977b). The example will illustrate how complex reaction kinetics can be programmed into the BLTM model. The coefficients for distributed sources (S_i) and the reaction coefficients $K_{i,n}$ are determined in a subroutine called FINK. The FORTRAN coding for the subroutine is stored in a file called QUAL2.F77 and a listing of the code is given in figure 11. The QUAL-II version of FINK computes all decay coefficients based on data contained in an input file called QUAL2.IN. QUAL2.IN contains all user-defined coefficients as well as a time series of meteorologic data. The format for the data in file QUAL2.IN is illustrated in Appendix B. Meteorologic data should represent average conditions during the time step. The water temperature in QUAL2.F77 is computed with Jobson's (1981) simplified temperature algorithm. This variation to the computational approach used by Roesner and others (1977a, 1977b) greatly simplifies the input data and is believed to be as accurate (Schoellhamer and Jobson, 1986b).

The file QUAL2.IN is shown in figure 12 and the file format is given in Appendix B. All rate coefficients are assumed uniform throughout the network but most values can vary from reach to reach. All values have been assumed to fall within the range recommended by Roesner and others (1977a, 1977b). The equilibrium temperature and wind speed (first two values on the TIME cards) were assumed constant at all times but the solar radiation is assumed to be zero until 6 AM (time 6) and after 6:00 PM.

Figure 13 contains a listing of the output file BLTM.OUT for this example. The output first lists self-explanatory simulation control information. Output is given at branch 2 grid point 1 and branch 3 grid point 3 every 6 hours. The time variation in the concentration of dissolved oxygen at these two grid points will be discussed in some detail in order to illustrate interpretation of the output.

The flow at branch 2 grid point 1 is zero so the initial parcel remains at this location for the entire simulation as indicated by the constant PH of -1.00. The volume of the parcel (PV) remains constant at $2.98 \times 10^5 \text{ m}^3$ until hour 18:00.

Between 18:00 hours and 24:00 hours the parcel volume is reduced to $2.95 \times 10^5 \text{ m}^3$ indicating that during the simulation slightly more volume was removed from the branch during the time of positive flow than entered the branch during the initial period of negative flow (see figure 7).

Applying the decay coefficients set in QUAL2.F77 (figure 11) under the heading DISSOLVED OXYGEN to equation 3, it is seen that the governing equation for dissolved oxygen is

$$\frac{\partial(\text{OXYG})}{\partial t} = \text{DIS} + S_8 + XK_{8,2} \text{ ALGE} + XK_{8,3} \text{ NH}_3 + XK_{8,4} \text{ NO}_2 + XK_{8,7} \text{ BOD} + XK_{8,8} (\text{OXYG} - \text{CR}_{8,8}), \quad (9)$$

Figure 11.--Listing of subroutine FINK containing
QUAL-II kinetics.

```

C
C*****CALCULATE THE CONSTITUENT COEFFICIENTS*****
C
C      SUBROUTINE FINK (K,MX,J,NEQ,PV,PT,
C      $ Q,A,W,XK,S,CR,IRC,NNN,LUOUT)
C
C      DEFINE VARIABLES:
C
C      NAME                PURPOSE
C      -----
C      A  AVERAGE AREA OF THE SUBREACH [SQ M]
C      CR(E,L) REFERENCE (EQUILIBRIUM) CONCENTRATION IN EQUATION E FOR
C             CONSTITUENT L
C      J    TIME STEP
C      K    PARCEL NUMBER
C      MX   GRID JUST UPSTREAM OF PARCEL'S UPSTREAM BOUNDRY
C      NEQ  NUMBER OF EQUATIONS (CONSTITUENTS)
C      NBRCH NUMBER OF BRANCHES
C      NXSEC(N) NUMBER OF SUBREACHES IN BRANCH N
C      NNN  BRANCH NUMBER
C      IENG input units: 0=metric, 1=English
C      IRC  CODE TO SET READ FOR NEW DATA EACH TIME STEP
C      PT(L,K) CONCENTRATION ON CONSTITUENT L IN PARCEL K
C      S(L)  SOURCE FLUX OF CONSTITUENT L [UNITS PER HOUR]
C      TE   Equilibrium water temperature, degrees C
C      V    Wind speed in meters/second
C      W    AVERAGE TOP WIDTH OF THE SUBREACH [M]
C      XK(L,LL) EXCHANGE COEFFICIENT FOR CONSTITUENT L DUE TO THE
C             CONCENTRATION OF CONSTITUENT LL
C      GROMAX MAXIMUM SPECIFIC GROWTH RATE OF ALGAE [PER DAY]
C      CKN  NITROGEN HALF-SATURATION CONSTANT FOR ALGAE [MG/L]
C      CKP  PHOSPHORUS HALF-SATURATION CONST. FOR ALGAE [MG/L]
C      EXCOEF= LIGHT EXTINCTION COEF.FOR ALGAE [PER METER]
C      CKL  LIGHT HALF-SATURATION CONST.FOR ALGAE [LANGLEY/MIN]
C      SONET LIGHT INTENSITY [LANGLEY/MIN]
C      RESPT ALGAE RESPIRATION RATE [PER DAY]
C      ALGSET(N,I)=LOCAL SETTLING RATE FOR ALGAE [M/DAY]
C      ALPHA1=FRACTION OF ALGAE WHICH IS NITROGEN
C      CKNH3(N,I)= RATE CONSTANT FOR BIOLOGICAL OXIDATION OF NH3 TO NO3
C             IN PER DAY
C      SNH3(N,I)=BENTHOS SOURCE RATE FOR NH3 [GM-N/DAY M]
C      CKNO2(N,I)=RATE CONSTANT FOR BIOLOGICAL OXIDATION OF NO2-NO3
C             [PER DAY]
C      ALPHA3=OXYGEN PRODUCTION PER UNIT OF ALGAE GROWTH
C      ALPHA2=FRACTION OF ALGAE BIOMASS THAT IS PHOSPHORUS
C      ALPHA4=OXYGEN UPTAKE PER UNIT OF ALGAE EXPIRED
C      ALPHA5=OXYGEN UPTAKE PER UNIT OF NH3 OXIDATION
C      ALPHA6=OXYGEN UPTAKE PER UNIT OF NO2 OXIDATION
C      SPHOS(N,I)=BENTHOS SOURCE RATE FOR PHOSPHORUS [GRAM/DAY M]
C      CK1(N,I)=CARBONACEOUS BOD DECAY RATE [PER DAY]
C      CK3(N,I)=CARBONACEOUS BOD SINK RATE [PER DAY]
C      CK2(N,I)=REAERATION RATE [PER DAY]
C      CK4(N,I)=BENTHOS CONSUMPTION OF OXYGEN [GM/DAY M]
C      CK5(N,I)=COLIFORM DIE-OFF RATE [PER DAY]
C      CK6(N,I)=ARBITRARY NON-CONSERVATIVE DECAY RATE [PER DAY]
C      A1=CONSTANT IN WIND FUNCTION [MM/DAY KPA] SUGEST 3.01
C      B1=MASS TRANSFER COEF [MM/DAY KPA(M/S)] SUGEST 1.13
C

```

```

C*** BEGIN DIMENSIONING DEFINITION
C
C NOBR Maximum number of branches allowed in model
C NOSC Maximum number of cross sections (grids) allowed in branch
C NOPR Maximum number of parcels allowed in branch
C (NOPR should be at least 20 + 2 times NOSC)
C NOCO Maximum number of constituents allowed
C
INTEGER NOBR,NOSC,NOPR,NOCO
PARAMETER (NOBR=30, NOSC=19, NOPR=26, NOCO=10)
C
C + + + LOCAL VARIABLES + + +
INTEGER I, I1, IRC, J, K, LUOUT, LUQ2, MX, NEQ, NNN, NXSEC (NOBR)
REAL CKNH3 (NOBR, NOSC), CKNO2 (NOBR, NOSC), ALGSET (NOBR, NOSC),
# SPHOS (NOBR, NOSC), SNH3 (NOBR, NOSC), CK1 (NOBR, NOSC),
# CK2 (NOBR, NOSC), CK3 (NOBR, NOSC), CK4 (NOBR, NOSC),
# CK5 (NOBR, NOSC), CK6 (NOBR, NOSC), XK (NOCO, NOCO),
# S (NOCO), CR (NOCO, NOCO), PT (NOCO, NOPR)
COMMON NXSEC, NBRCH, IENG
SAVE CKNH3, CKNO2, ALGSET, SPHOS, SNH3, GROMAX, RESPRT,
1 CKN, CKP, CKL, EXCOEF, SONE, A1, B1, TE, V
2 ALPHA1, ALPHA2, ALPHA3, ALPHA4, ALPHA5, ALPHA6
3 CK1, CK2, CK3, CK4, CK5, CK6
IF (IRC.NE.1) GO TO 3
IF (J.NE.1) GO TO 2
LUQ2=19
OPEN (LUQ2, FILE='QUAL2.IN')
WRITE (LUOUT, 6000)
6000 FORMAT(/, 30X, 'Reaction Kinetics')
READ (LUQ2, 3305) A1, B1, GROMAX, CKN, CKP, EXCOEF, CKL, RESPRT
WRITE (LUOUT, 6001)
6001 FORMAT(/, ' TEMPERATURE')
WRITE (LUOUT, 6002) A1, B1
6002 FORMAT(' WIND FUNCTION=', F6.2, '+', F6.2, 'V [MM/DAY KPA WHEN V I
$N M/S].')
WRITE (LUOUT, *) 'ALGAE'
WRITE (LUOUT, 6003) GROMAX
6003 FORMAT(' MAXIMUM SPECIFIC GROWTH RATE=', F7.3, ' [PER DAY].')
WRITE (LUOUT, 6004) RESPRT
6004 FORMAT(' ALGAE RESPIRATION RATE =', F7.3, ' [PER DAY].')
WRITE (LUOUT, 6005) CKN
6005 FORMAT(' NITROGEN HALF-SAT. CONSTANT =', F7.3, ' [MGL/L].')
WRITE (LUOUT, 6006) CKP
6006 FORMAT(' PHOSPHORUS HALF-SAT. CONST. =', F7.3, ' [MGL/L].')
WRITE (LUOUT, 6007) EXCOEF
6007 FORMAT(' LIGHT EXTINCTION COEF. =', F7.3, ' [PER METER].')
READ (LUQ2, 3305) ALPHA1, ALPHA2, ALPHA3, ALPHA4, ALPHA5, ALPHA6
3305 FORMAT(10X, 10F7.3)
WRITE (LUOUT, 6008) ALPHA1
6008 FORMAT(' FRACTION OF NITROGEN/ALGAE =', F7.3, ' .')
WRITE (LUOUT, 6009) ALPHA2
6009 FORMAT(' FRACTION PHOSPHORUS/ALGAE =', F7.3, ' .')
WRITE (LUOUT, 6010) ALPHA3
6010 FORMAT(' OXYGEN PRODUCTION/GROWTH =', F7.3, ' .')
WRITE (LUOUT, 6011) ALPHA4
6011 FORMAT(' OXYGEN UPTAKE/EXPIRATION =', F7.3, ' .')
WRITE (LUOUT, 6012) ALPHA5
6012 FORMAT(' OXYGEN USED TO OXIDIZE NH3 =', F7.3, ' .')
WRITE (LUOUT, 6013) ALPHA6
6013 FORMAT(' OXYGEN USED TO OXIDIZE NO2 =', F7.3, ' .')
WRITE (LUOUT, 6014)
6014 FORMAT(' BR GRID ALGSET NH3-DECAY BNTHO-NH3 NO2-DECAY BNTHO-P
$HO K1 BOD-SINK K2 BNTHO-OXY COLI-DIE ARB-RATE')
WRITE (LUOUT, 6015)

```

```

6015 FORMAT(10X, '      M/DAY PER DAY GM/DAY M PER DAY GM/DAY M P
$ER DAY PER DAY PER DAY GM/DAY M PER DAY PER DAY')
DO 1 N=1, NBRCH
  I1=NXSEC(N)-1
  DO 1 I=1, I1
    READ(LUQ2, 3305)ALGSET(N, I), CKNH3(N, I), SNH3(N, I), CKNO2(N, I),
$ SPHOS(N, I)
    READ(LUQ2, 3305)CK1(N, I), CK2(N, I), CK3(N, I), CK4(N, I), CK5(N, I),
# CK6(N, I)
    IF(I.EQ.1)WRITE(LUOUT, 6016)N, I, ALGSET(N, I), CKNH3(N, I), SNH3(N, I),
$ CKNO2(N, I), SPHOS(N, I), CK1(N, I), CK3(N, I), CK2(N, I), CK4(N, I),
% CK5(N, I), CK6(N, I)
6016 FORMAT(2I5, 11F10.3)
  IF(I.GT.1)WRITE(LUOUT, 6017)I, ALGSET(N, I), CKNH3(N, I), SNH3(N, I),
$ CKNO2(N, I), SPHOS(N, I), CK1(N, I), CK3(N, I), CK2(N, I), CK4(N, I),
% CK5(N, I), CK6(N, I)
6017 FORMAT(5X, I5, 11F10.3)
1 CONTINUE
2 CONTINUE
  IF(IRC.NE.1)GO TO 3
  READ(LUQ2, 3305)TE, V, SONET
  WRITE(LUOUT, *)J, TE, V, SONET
3 CONTINUE
C
C TEMPERATURE (SIMPLIFIED TEMPERATURE ALGORITHM)
C
  IF(IENG.EQ.0)THEN
    AL=0.3048*0.3048*A
    WL=0.3048*W
  ELSE
    AL=A
    WL=W
  END IF
  CPR= 100.0
  SIG= 1.171E-7/24.0
  AL= 595.9-0.545*PT(1, K)
  PSI= (A1+B1*V)/(24.0*10.0)
  TAB= PT(1, K)+273.16
  DFT=1.1532E11*EXP(-4271.1/(PT(1, K)+242.63))
1 /((PT(1, K)+242.63)**2)
  XKK= 4.0*0.97*SIG*(TAB**3)+AL*PSI*(DFT+0.06)
  XK(1, 1)=0.0
  IF(A.GT.0.0)XK(1, 1)= -XKK*WL/(AL*CPR)
  CR(1, 1)=TE
C
C ALGAE
C
  XK(2, 2)=0.0
  IF(A.LE.0.0)GO TO 5
  DEXCOF=EXCOEF*AL/WL
  GRO=GROMAX*1.047**(PT(1, K)-20.0)
  IGRO=IFIX(PT(5, K)+CKN)
  IF(IGRO.NE.0)GRO=GRO*(PT(5, K)/(PT(5, K)+CKN))
1 *(PT(6, K)/(PT(6, K)+CKP))*(1.0/DEXCOF)
2 *LOG((CKL+SONET)/(CKL+SONET*EXP(-DEXCOF)))
C
  TRSPRT=RESPRT*1.047**(PT(1, K)-20.0)
  XK(2, 2)=(GRO-TRSPRT-ALGSET(NNN, MX)*WL/AL)/24.0
C
C AMMONIA NITROGEN

```

```

C
5 XK(3,2)=ALPHA1*TRSPRT/24.0
  XK(3,3)=- (CKNH3(NNN,MX)*1.047**(PT(1,K)-20.0))/24.0
  IF (PT(8,K).GT.0.0)XK(3,3)=XK(3,3)*(1.0-EXP(-PT(8,K)))
  IF (PT(8,K).LT.0.0)XK(3,3)=0.0
  IF (A.GT.0.0)S(3)=SNH3(NNN,MX)/(AL*24.0)
C
C   NITRITE NITROGEN
C
  XK(4,3)=-XK(3,3)
  XK(4,4)=0.0
  IF (A.GT.0.0)XK(4,4)=-CKNO2(NNN,MX)*1.047**(PT(1,K)-20.0)/24.0
  IF (PT(8,K).GT.0.0)XK(4,4)=XK(4,4)*(1.0-EXP(-PT(8,K)))
  IF (PT(8,K).LT.0.0)XK(4,4)=0.0
C
C   NITRATE NITROGEN
C
  XK(5,2)=-ALPHA1*GRO/24.0
  XK(5,4)=-XK(4,4)
C
C   DISSOLVED OROPHOSPHATE
C
  XK(6,2)=ALPHA2*(TRSPRT-GRO)/24.0
  S(6)=0.0
  IF (A.GT.0.0)S(6)=SPHOS(NNN,MX)/(AL*24.0)
C
C   BOD
C
  TCK1=CK1(NNN,MX)*1.047**(PT(1,K)-20.0)
  IF (PT(8,K).GT.0.0)TCK1=TCK1*(1.0-EXP(-PT(8,K)))
  IF (PT(8,K).LT.0.0)TCK1=0.0
  XK(7,7)=- (TCK1+CK3(NNN,MX))/24.0
C
C   DISSOLVED OXYGEN
C
  PTF=PT(1,K)*1.8+32.0
  CR(8,8)=24.89+PTF*(-0.426+PTF*(0.00373-PTF*0.0000133))
  XK(8,8)=- (CK2(NNN,MX)*1.0159**(PT(1,K)-20.0))/24.0
  XK(8,7)=-TCK1/24.0
  XK(8,3)=ALPHA5*XK(3,3)
  XK(8,2)=(ALPHA3*GRO-ALPHA4*TRSPRT)/24.0
  XK(8,4)=ALPHA6*XK(4,4)
  S(8)=0.0
  IF (A.GT.0.0)S(8)=-CK4(NNN,MX)/(24.0*AL)
C
C   COLIFORM
C
  XK(9,9)=0.0
  IF (A.GT.0.0)XK(9,9)=-CK5(NNN,MX)*1.047**(PT(1,K)-20.0)/24.0
C
C   ARBITRARY NONCONSERVATIVE CONSTITUENT
C
  XK(10,10)=- (CK6(NNN,MX)*1.047**(PT(1,K)-20.0))/24.0
  IRC=0
  RETURN
  END

```

HEADER 1	3.01	1.13	2.0	0.3	0.04	0.1	0.03	0.2
HEADER 2	0.08	0.012	1.6	2.0	3.43	1.14		
B1 S 1	1.5	0.3	3.6	1.5	6.0			
B1 S 1	1.10	4.0	0.24	0.6	1.8	0.0		
B1 S 2	1.5	0.3	3.6	1.5	6.0			
B1 S 2	1.10	4.0	0.24	0.6	1.8	0.0		
B1 S 3	1.5	0.3	3.6	1.5	6.0			
B1 S 3	1.10	4.0	0.24	0.6	1.8	0.0		
B2 S 1	1.5	0.3	3.6	1.5	6.0			
B2 S 1	1.10	4.0	0.24	0.6	1.8	0.0		
B2 S 2	1.5	0.3	3.6	1.5	6.0			
B2 S 2	1.10	4.0	0.24	0.6	1.8	0.0		
B3 S 1	1.5	0.3	3.6	1.5	6.0			
B3 S 1	1.10	4.0	0.24	0.6	1.8	0.0		
B3 S 2	1.5	0.3	3.6	1.5	6.0			
B3 S 2	1.10	4.0	0.24	0.6	1.8	0.0		
B3 S 3	1.5	0.3	3.6	1.5	6.0			
B3 S 3	1.10	4.0	0.24	0.6	1.8	0.0		
B3 S 4	1.5	0.3	3.6	1.5	6.0			
B3 S 4	1.10	4.0	0.24	0.6	1.8	0.0		
B3 S 5	1.5	0.3	3.6	1.5	6.0			
B3 S 5	1.10	4.0	0.24	0.6	1.8	0.0		
B3 S 6	1.5	0.3	3.6	1.5	6.0			
B3 S 6	1.10	4.0	0.24	0.6	1.8	0.0		
B4 S 1	1.5	0.3	3.6	1.5	6.0			
B4 S 1	1.10	4.0	0.24	0.6	1.8	0.0		
B4 S 2	1.5	0.3	3.6	1.5	6.0			
B4 S 2	1.10	4.0	0.24	0.6	1.8	0.0		
B4 S 3	1.5	0.3	3.6	1.5	6.0			
B4 S 3	1.10	4.0	0.24	0.6	1.8	0.0		
B5 S 1	1.5	0.3	3.6	1.5	6.0			
B5 S 1	1.10	4.0	0.24	0.6	1.8	0.0		
B5 S 2	1.5	0.3	3.6	1.5	6.0			
B5 S 2	1.10	4.0	0.24	0.6	1.8	0.0		
B6 S 1	1.5	0.3	3.6	1.5	6.0			
B6 S 1	1.10	4.0	0.24	0.6	1.8	0.0		
B6 S 2	1.5	0.3	3.6	1.5	6.0			
B6 S 2	1.10	4.0	0.24	0.6	1.8	0.0		
TIME 1	20.0	3.0	0.0					
TIME 2	20.0	3.0	0.0					
TIME 3	20.0	3.0	0.0					
TIME 4	20.0	3.0	0.0					
TIME 5	20.0	3.0	0.0					
TIME 6	20.0	3.0	0.0					
TIME 7	20.0	3.0	0.31					
TIME 8	20.0	3.0	0.6					
TIME 9	20.0	3.0	0.85					
TIME 10	20.0	3.0	1.04					
TIME 11	20.0	3.0	1.16					

Figure 12.--Input file QUAL2.IN for the QUAL-II example
(Continued on next page.)

TIME	12	20.0	3.0	1.2
TIME	13	20.0	3.0	1.16
TIME	14	20.0	3.0	1.04
TIME	15	20.0	3.0	0.85
TIME	16	20.0	3.0	0.6
TIME	17	20.0	3.0	0.31
TIME	18	20.0	3.0	0.0
TIME	19	20.0	3.0	0.0
TIME	20	20.0	3.0	0.0
TIME	21	20.0	3.0	0.0
TIME	22	20.0	3.0	0.0
TIME	23	20.0	3.0	0.0
TIME	24	20.0	3.0	0.0

Figure 12.--Input file QUAL2.IN for the QUAL-II example
(Continued.)

Figure 13.--Output file BLTM.OUT for the QUAL-II Example

THE 6 BRANCH MODEL WITH 2 INTERNAL JUNCTIONS IS RUN 24 TIME STEPS EACH 1.00 HOURS LONG.
 THE MODEL STARTS AT 0.00 HOURS PAST MIDNIGHT.
 THE GRID OUTPUT IS GIVEN IN BLTM.OUT EVERY 6 TIME STEPS.
 THE PARCEL OUTPUT IS GIVEN IN PARCEL.OUT EVERY 6 TIME STEPS.
 10 CONSTITUENTS ARE ROUTED AND THE MINIMUM DISPERSIVE VELOCITY IS 0.100 M/S.
 BOUNDARY CONDITIONS ARE READ FROM BLTM.IN
 FLOW FIELD READ FROM BLTM.FLW
 INPUT UNITS ARE METRIC (METERS) EXCEPT RIVER MILES

INITIAL CONDITIONS

GRID MILE	RIVER DISCHARGE CU M/S	AREA SQ M	TOP WIDTH METERS	TRIB. FLOW CU M/S	TEMP	ALGE	NH3	INITIAL CONCENTRATION					BOD	OXYG	COLI	ARB
								NO2	NO3	PHOS	PHOS	PHOS				
BRANCH 1 DQQ= 0.30 EXTENDS FROM JUCT 3 TO JUNCTION 1																
1	0.00	30.00	356.52	164.04	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
2	0.30	28.19	356.37	164.04	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
3	0.61	36.31	356.30	164.04	0.00											
BRANCH 2 DQQ= 0.30 EXTENDS FROM JUCT 4 TO JUNCTION 1																
1	0.00	0.00	130.11	60.00	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
2	1.42	-3.30	130.32	60.00	0.00											
BRANCH 3 DQQ= 0.30 EXTENDS FROM JUCT 1 TO JUNCTION 2																
1	0.00	17.48	206.86	95.24	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
2	0.47	15.33	226.97	104.74	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
3	0.95	12.30	247.28	114.29	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
4	1.42	8.71	268.10	123.81	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
5	1.89	5.53	288.73	133.33	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
6	2.37	1.94	309.36	142.86	0.00											
BRANCH 4 DQQ= 0.30 EXTENDS FROM JUCT 1 TO JUNCTION 2																
1	0.00	5.58	78.20	36.00	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
2	0.85	4.50	77.91	36.00	0.00	10.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	10.00
3	1.70	2.98	77.96	36.00	0.00											

Continued on next page

Figure 13.--Output file BLTM.OUT for the QUAL-II Example (Continued)

BRANCH	5	DQQ=	0.30	EXTENDS FROM JUCT 2 TO JUNCTION 5
1	0.00	12.02	108.27	50.00
2	1.04	7.14	106.25	50.00
BRANCH	6	DQQ=	0.30	EXTENDS FROM JUCT 2 TO JUNCTION 6
1	0.00	-7.10	126.32	58.33
2	1.04	-12.65	129.21	58.33

Reaction Kinetics

TEMPERATURE
WIND FUNCTION= 3.01+ 1.13V [MM/DAY KPA WHEN V IN M/S].
ALGAE

- MAXIMUM SPECIFIC GROWTH RATE= 2.000 [PER DAY].
- ALGAE RESPIRATION RATE = 0.200 [PER DAY].
- NITROGEN HALF-SAT. CONSTANT = 0.300 [MGL/L].
- PHOSPHORUS HALF-SAT. CONST. = 0.040 [MGL/L].
- LIGHT EXTINCTION COEF. = 0.100 [PER METER].
- FRACTION OF NITROGEN/ALGAE = 0.080 .
- FRACTION PHOSPHORUS/ALGAE = 0.012 .
- OXYGEN PRODUCTION/GROWTH = 1.600 .
- OXYGEN UPTAKE/EXPIRATION = 2.000 .
- OXYGEN USED TO OXIDIZE NH3 = 3.430 .
- OXYGEN USED TO OXIDIZE NO2 = 1.140 .

BR GRID	ALGSET	NH3-DECAY	BNTHO-NH3	NO2-DECAY	BNTHO-PHO	K1	BOD-SINK	K2	BNTHO-OXY	COLI-DIE	ARB-RATE
	M/DAY	PER DAY	GM/DAY M	PER DAY	GM/DAY M	PER DAY	PER DAY	PER DAY	GM/DAY M	PER DAY	PER DAY
1	1	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
	2	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
	3	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
2	1	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
	2	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
	3	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
3	1	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
	2	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
	3	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800
4	1.500	0.300	3.600	1.500	6.000	6.000	1.100	0.240	4.000	0.600	1.800
5	1.500	0.300	3.600	1.500	6.000	6.000	1.100	0.240	4.000	0.600	1.800
6	1.500	0.300	3.600	1.500	6.000	6.000	1.100	0.240	4.000	0.600	1.800

Continued on next page

Figure 13.--Output file BLTM.OUT for the QUAL-II Example (Continued)

4	1	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800	0.000				
	2	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800	0.000				
	3	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800	0.000				
5	1	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800	0.000				
	2	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800	0.000				
6	1	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800	0.000				
	2	1.500	0.300	3.600	1.500	6.000	1.100	0.240	4.000	0.600	1.800	0.000				
DAY	1	HOUR 6.0	VU	TEMP	ALGE	NH3	NO2	NO3	PHOS	BOD	OXYG	COLI	ARB			
BR	2	GRID 1	K= 1	0.000	0.298E+06	-1.00	10.959	1.647	2.869	3.265	5.877	6.011	5.520	7.974	6.728	10.000
					PVI		10.000	2.000	3.000	4.000	5.000	6.000	7.000	8.000	9.000	10.000
					PDF		0.286	0.001	-0.001	-0.002	0.002	0.000	-0.001	-0.034	-0.006	0.000
					PDC		0.673	-0.354	-0.142	-0.875	0.000	0.001	-1.478	-0.115	-2.266	0.000
BR	3	GRID 3	K= 8	0.987E+05	0.181E+06	-2.00	10.765	1.648	2.867	3.273	5.868	6.006	5.533	8.008	6.751	10.000
					PVI		10.000	2.000	3.000	4.000	5.000	6.000	7.000	8.000	9.000	10.000
					PDF		0.088	0.003	0.001	0.004	-0.004	0.000	0.008	-0.014	0.011	0.000
					PDC		0.677	-0.354	-0.141	-0.872	0.000	0.001	-1.475	-0.115	-2.260	0.000
DAY	1	HOUR 12.0	VU	TEMP	ALGE	NH3	NO2	NO3	PHOS	BOD	OXYG	COLI	ARB			
BR	2	GRID 1	K= 1	0.000	0.298E+06	-1.00	12.153	1.875	2.733	2.644	6.602	6.015	4.297	8.561	4.919	10.000
					PVI		10.000	2.000	3.000	4.000	5.000	6.000	7.000	8.000	9.000	10.000
					PDF		0.918	0.011	-0.004	-0.016	0.019	-0.001	-0.019	-0.159	-0.047	0.000
					PDC		1.235	-0.137	-0.285	-1.625	-0.044	-0.005	-2.685	0.637	-4.034	0.000
BR	3	GRID 3	K= 7	0.276E+05	0.451E+05	6.00	19.276	2.227	2.686	2.489	6.773	6.000	4.141	7.141	4.491	10.000
					PVI		21.230	1.732	2.856	3.231	5.919	6.003	5.572	6.448	6.630	10.000
					PDF		-2.017	0.027	0.020	0.085	-0.106	0.000	0.135	0.428	0.246	0.000
					PDC		0.063	0.468	-0.201	-1.028	-0.070	-0.009	-1.565	1.202	-2.385	0.000
DAY	1	HOUR 18.0	VU	TEMP	ALGE	NH3	NO2	NO3	PHOS	BOD	OXYG	COLI	ARB			
BR	2	GRID 1	K= 1	0.000	0.298E+06	-1.00	13.108	2.040	2.598	2.134	7.215	6.019	3.306	8.817	3.530	10.000
					PVI		10.000	2.000	3.000	4.000	5.000	6.000	7.000	8.000	9.000	10.000
					PDF		1.336	0.033	-0.009	-0.032	0.038	-0.001	-0.040	-0.251	-0.091	0.000
					PDC		1.772	0.007	-0.428	-2.262	-0.087	-0.011	-3.654	1.357	-5.379	0.000
BR	3	GRID 3	K= 5	0.406E+05	0.985E+05	14.00	23.344	2.866	2.631	2.301	6.954	5.991	3.861	6.583	4.003	10.000
					PVI		23.685	2.542	2.791	2.946	6.198	5.994	5.069	6.851	5.809	10.000
					PDF		-0.090	0.010	-0.013	-0.049	0.060	0.000	-0.094	0.017	-0.134	0.000
					PDC		-0.251	0.314	-0.158	-0.754	-0.060	-0.008	-1.114	0.970	-1.672	0.000
DAY	2	HOUR 0.0	VU	TEMP	ALGE	NH3	NO2	NO3	PHOS	BOD	OXYG	COLI	ARB			
BR	2	GRID 1	K= 1	0.000	0.295E+06	-1.00	13.719	1.661	2.468	1.736	7.753	6.031	2.536	8.542	2.524	10.000
					PVI		10.000	2.000	3.000	4.000	5.000	6.000	7.000	8.000	9.000	10.000
					PDF		1.415	0.038	-0.010	-0.036	0.043	-0.002	-0.046	-0.270	-0.100	0.000
					PDC		2.305	-0.377	-0.568	-2.796	-0.087	-0.010	-4.418	1.223	-6.376	0.000
BR	3	GRID 3	K= 5	0.147E+05	0.963E+05	20.00	23.382	1.724	2.647	2.384	6.955	6.007	4.013	5.592	4.237	10.000
					PVI		23.641	1.918	2.817	3.076	6.095	6.003	5.301	6.340	6.201	10.000
					PDF		0.009	0.092	-0.019	-0.070	0.078	-0.001	-0.130	0.030	-0.190	0.000
					PDC		-0.268	-0.286	-0.159	-0.781	0.000	0.001	-1.158	-0.142	-1.774	0.000

in which DIS represents the dispersion and the other terms are defined in figure 11 or Appendix B. The oxygen source terms (S_8), for example, is defined in Figure 11 as

$$S_8 = -A CK4_{n,i}/24.0, \quad (10)$$

in which CK4 is the benthic source rate for BOD in gram day⁻¹ m⁻¹ for branch n and reach i (0.60, Fig. 13) and A is the cross-sectional area of branch n reach i. The constant 24 converts the units of per day to per hour. The units of S_8 are mass per cubic meter per hour. The negative indicates the benthos consumes oxygen rather than produces it. The production rate of oxygen by algae ($XK_{8,2}$) is given by

$$XK_{8,2} = (\text{ALPHA3} * \text{GRO} - \text{ALPHA4} * \text{TRSPRT}) / 24, \quad (11)$$

in which ALPHA3 (1.60) is the oxygen produced per unit of algae growth, GRO is the growth rate of oxygen (computed in the decay coefficient subroutine) ALPHA4 (2.0) is the oxygen uptake per unit of algae expired and TRSPRT is the algae respiration rate (0.2 per day) corrected for water temperature. Again the constant 24 converts the units from per day to per hour. $XK_{8,3}$, $XK_{8,4}$, and $XK_{8,7}$ are reaction rates for NH₃ oxidation, NO₂ oxidation, and BOD decay. Finally the last term in equation 9 represents reaeration. The reaeration rate $XK_{8,8}$ is computed as

$$XK_{8,8} = \frac{(-CK2_{n,i} 1.0159^{(\text{TEMP}-20)})}{24} \quad (12)$$

in which CK2 is the reference reaeration coefficient in branch n subreach i (input as 4.0 per day) corrected for the local water temperature and the minus sign is present because oxygen deficit is given by $(C_8 - CR_{8,8}) < 0$. The equilibrium concentration of dissolved oxygen ($CR_{8,8}$) is the saturation concentration given by

$$CR_{8,8} = 24.89 - 0.426 \text{ PTF} + 0.00373 \text{ PTF}^2 - 0.0000133 \text{ PTF}^3, \quad (13)$$

in which PTF is the local temperature expressed in Fahrenheit degrees.

The model allows one to determine the effect of each of the terms in equation 9 on the final oxygen concentration as will be illustrated below.

Consider the parcel at grid point 1 in branch 2 at the end of the simulation, after 24 hours of remaining stationary. The output in figure 13 indicates that the parcel started with 8.000 mg/L of oxygen (PTI) and ended up with a concentration of 8.542 mg/L for a net increase of 0.542 mg/L. It may be of interest to determine what processes contributed to this change. Figure 13 indicates that during the 24 hours dispersion decreased its concentration by 0.270 mg/L (PDF) and algae added 1.223 mg/L (PDC). It is known that the value of PDC in figure 13 represents the net production by algae because $LR_8 = 2$ in figure 10 and PDC is computed from equation 7. The contribution of each of the terms in equation 9 can be quantified by rerunning the model with various values of LR_i . This was done and the results tabulated in table 2. The benthic consumption term (S_8) was determined as the difference between the final and initial concentration after accounting for all other terms. Looking at the table for hour 24, branch 2, grid point 1, it is seen that several processes had a significant effect even though the total net change was small.

For example, reaeration added 8.101 mg/L of oxygen and BOD consumed 3.282 mg/L. Nitrification consumed 1.941 mg/L in converting ammonia to nitrite and 3.134 mg/L in converting nitrite to nitrate. Algae growth produced a net of 1.223 mg/L and benthos consumed only 0.155 mg/L. The effect of algae on the dissolved oxygen was quite variable throughout the day. As can be seen, respiration consumed 0.115 mg/L between midnight and 6 AM when the growth rate was zero but photosynthesis produced a net of 1.472 mg/L (1.357 - (-0.115)) from 6 AM to 6 PM.

It should be emphasized that the term PDC accumulates the effect of reaction kinetics only during the time the parcel is in a branch. For example, the parcel at branch 3 grid point 3 at hour 12 entered the branch at hour 6.00 (PH = 6.00) so the travel time (TT) in branch 3 was 6 hours and algal photosynthesis produced 1.202 mg/L of oxygen during this 6 hour period. The parcel at branch 3 grid point 3 at hour 24 entered the branch at hour 20 so the algal production of oxygen in this parcel of -0.142 mg/L represents respiration during the 4 hours from 2000 hours to 2400 hours. During the four hour time span the parcel concentration of dissolved oxygen decreased from 6.339 (PTI = 6.339) to 5.591 (PT = 5.591) mg/L.

Programs CTPLT.F77 and CXPLT.F77 could be used to plot the variation of concentration with time or the instantaneous concentration profiles, respectively, for any of the ten constituents using data stored in PARCEL.OUT.

Table 2.--Contribution of each term in equation 9 to the final concentration of oxygen for parcels at two grid points

Branch	Grid	PH	TT	OXYG	PTI	PDF	ALGAE 2	NH3 3	NO2 4	BOD 7	OXY 8	S _g
hour 6												
2	1	-1	6	7.974	8.000	-0.034	-0.115	-0.485	-0.980	-1.082	2.715	-0.045
3	3	-2	6	8.008	8.000	-0.014	-0.115	-0.483	-0.978	-1.079	2.719	-0.042
hour 12												
2	1	-1	12	8.561	8.000	-0.159	0.637	-0.973	-1.821	-1.977	4.943	-0.089
3	3	6	6	7.141	6.448	0.428	1.202	-0.685	-1.147	-1.246	2.222	-0.081
hour 18												
2	1	-1	18	8.817	8.000	-0.251	1.357	-1.461	-2.534	-2.703	6.538	-0.129
3	3	14	4	6.583	6.850	0.017	0.970	-0.541	-0.841	-0.917	1.111	-0.066
hour 24												
2	1	-1	24	8.542	8.000	-0.270	1.223	-1.941	-3.134	-3.282	8.101	0.155
3	3	20	4	5.591	6.339	0.030	-0.142	-0.543	-0.872	-0.953	1.781	-0.049
(Concentration units in mg/L)												

SUMMARY

A Users Manual for the Branched Lagrangian Transport Model (BLTM) has been presented. The BLTM uses Lagrangian calculations that are unconditionally stable and based upon a reference frame that moves at a velocity equal to the mean channel flow velocity. BLTM results are within the accuracy required by most water-quality studies. The BLTM is easily applied to unsteady and unstratified flows in networks of one-dimensional channels with fixed geometry and tributary inflows. Reaction kinetics for up to ten constituents are provided in a user-written decay-coefficient subroutine, examples of which are given for a conservative constituent and the QUAL-II water-quality model's reactions and constituents. Post-processor plot programs and the Time-Dependent Data System improve the utility of the model.

REFERENCES

- Jobson, H. E., 1985, Simulating unsteady transport of nitrogen, biochemical oxygen demand, and dissolved oxygen in the Chattahoochee River downstream from Atlanta, Georgia: U.S. Geological Survey Water Supply Paper, no. 2264, 36 p.
- _____ 1981, Temperature and solute-transport simulation in streamflow using a Lagrangian reference frame: U.S. Geological Survey, Water-Resources Investigations Report 81-2, 165 p.
- _____ 1980, Comment on A new collocation method for the solution of the convection-dominated transport equation, by Pinder, George E. and Shapiro, Allen, 1979, (*in Water Resources Research*, v. 15, no. 5, p. 1177-1182): *Water Resources Research*, v. 16, no. 6, p. 1135-1136.
- Proesner, L. A., Giguere, P. R., and Evenson, D. C., 1977a, Computer program documentation for the stream quality model QUAL-II: prepared by Water Resources Engineers Inc., Walnut Creek, Calif., for Southeast Michigan Council of Governments, Detroit, Michigan.
- _____ 1977b. Users manual for the stream quality model QUAL-II: prepared by Water Resources Engineers, Inc., Walnut Creek, Calif., for Southeast Michigan Council of Governments, Detroit, Michigan.
- Schaffranek, R. W., Baltzer, R. A., and Goldberg, D. E., 1981, A model for simulation of flow in singular and interconnected channels: *Techniques of Water-Resources Investigations of the U.S. Geological Survey*, Book 7, Chapter C3.
- Schoellhamer, D. H., and Jobson, H. E., 1986a, Programmers manual for a one-dimensional Lagrangian transport model: U.S. Geological Survey Water-Resources Investigation Report 86-4144, 101 p.
- _____ 1986b, Users manual for a one-dimensional Lagrangian transport model: U.S. Geological Survey Water-Resources Investigation Report 86-4145, 95 p.
- Thomson, N. R., Sykes, J. F., and Lennox, W. C., 1984, A Lagrangian porous media mass transport model: *Water Resources Research*, v. 20, no. 3, p. 391-399.

Appendix A

INPUT FILE FORMAT FOR BLTM.IN

Data Set 1 -- Simulation Title

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
1	TITLE	20A4	Title of Simulation

Data Set 2 -- Fixed Point Header

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
0		10X	Card label
1	NBRCH	I7	Number of branches to be simulated (MAXIMUM = 30)
2	NJNCT	I7	Number of interior junctions (MAXIMUM = 29)
3	NHR	I7	Number of time steps to be modeled
4	NEQ	I7	Number of constituents to be modeled (MAXIMUM = 10)
5	JTS	I7	Number of time steps between midnight and the start of the model
6	JGO	I7	Number of time steps between printouts in BLTM.OUT
7	JPO	I7	Number of time steps between printouts in PARCEL.OUT
8	ITDDS	I7	Code indicating use of TDDS (0 = Do not use TDDS, 1 = Read hydraulic data with TDDS, 2 = Read hydraulic and boundary condition data with TDDS, DEFAULT = 0)
9	IENG	I7	Input units [0 = metric (length unit is meters except for river miles), 1 = English (length unit is feet except river miles), DEFAULT = 0].
10			Empty

Data Set 3 -- Floating Point Header

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
0		10X	Card Label
1	DT	F7.0	Time step size in hours
2	DQV	F7.0	Minimum dispersive velocity in ft/s or m/s
3-10			Empty

Data Set 4 -- Constituent Labels

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
0		10X	Card label
1	L	17	Constituent number
2	LABEL(L)	3X,A4	Name of constituent (4 symbols maximum)
3	LR(L)	I7	Index denoting that the decay of constituent L due to the presence of constituent LR(L) is accumulated.
4-10			Empty

(One constituent label card for each constituent)

(Cards must be in order from constituent 1 to NEQ)

Data Set 5 -- Branch Information

Field	Variable	Format	Description
(Card 1 ~ header)			
0		10X	Card label for branch N
1	NXSEC(N)	I7	Number of grids in branch N
2	DQQ(N)	F7.0	Dispersion factor for branch N
3	JNCU(N)	I7	Junction number at upstream end of branch N
4	JNCD(N)	I7	Junction number at downstream end of branch N
5	INPR(N)	I7	Initial number of parcels per reach in branch N (DEFAULT = 1)
6-10			Empty
(Card 2 ~ Grid data for branch N)			
0		10X	Card label for Grid I of branch N
1	X(N,I)	F7.0	Distance of grid I from upstream end of branch N (JNCU(N)) in miles.
2	IOUT(N,I)	I7	Output flag (equal 1 if output in BLTM.OUT is desired for this grid, 0 otherwise)
3	GPT(N,I,1)	F7.0	Initial concentration of constituent 1 between grid I and I+1 (omit for I = NXSEC(N))
o	o		
o	o		
o	o		
10	GPT(N,I,8)	F7.0	Initial concentration of constituent 8 between grid I and I+1 (omit for I= NXSEC(N))

Data Set 5 -- Branch Information (Continued)

Field	Variable	Format	Description
			(Card 3 ~ Initial concentration of constituents 9 and 10 if needed) (Omit for I = NXSEC(N))
0		10X	Card label
1	GPT(N,I,9)	F7.0	Initial concentration of constituent 9 between grid I and I+1
2	GPT(N,I,10)	F7.0	Initial concentration of constituent 10 between I and I+1
3-10			Empty

(Repeat cards 2 and 3 for each grid in Branch N)

(Repeat cards 1, 2, and 3 for each Branch)

Branches must be input in sequence starting with branch 1

Data Set 6 -- TDDS Control Card

Include only if TDDS is used (ITDDS > 0)

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
0		10X	Card label
1	NINPUT	I7	Number of TDDS input data types for the simulation
2	NOUT	I7	Number of TDDS output time series for the simulation, MAXIMUM = 10
3	LIST	I7	DADIO list option: -Print calendar year and index directory summaries, LIST = -1 -Do not print summaries, LIST = 0 -Print only the index directory summary, LIST = 1
4-10			Empty

Data Set 7 -- TDDS Dates Card

Include only if TDDS is used (ITDDS > 0)

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
0		10X	Card label
1	BY	I7	Beginning year of simulation (i.e. for 1986 use 86)
2	BMO	I7	Beginning month of simulation
3	BD	I7	Beginning day of simulation
4	BH	I7	Beginning hour of simulation
5	BMN	I7	Beginning minute of simulation
6	EY	I7	Ending year of simulation (i.e. for 1986 use 86)
7	EMO	I7	Ending month of simulation
8	ED	I7	Ending day of simulation
9	EH	I7	Ending hour of simulation
10	EMN	I7	Ending minute of simulation

Data Set 8 -- TDDS Station Identification

Include only if TDDS is used (ITDDS > 0)

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
0		10X	Card label, on all cards in data set
1,2	STAID(N,1)	I14	TDDS station identification number for branch N, grid 1
3,4	STAID(N,2)	I14	TDDS station identification number for branch N, grid 2
.	.	.	.
.	.	.	.
.	.	.	.
2*NXSEC(N)-1, 2*NXSEC(N)	STAID(NXSEC(N))	I14	TDDS station identification number for branch N, grid NXSEC(N)

**Repeat data set for each branch (NBR times), where N = 1 to NBR.

Data Set 9 -- TDDS Input

Include only if NINPUT > 0

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
0		10X	Card label, on all cards in data set
1	INTYPE(I)	5X,A2	TDDS data type
2	RDPDY(I)	I7	Readings per day of INTYPE(I) in TDDS, DEFAULT = number of simulation time steps per day
3	NINGRD(I)	I7	Number of grids with INTYPE(I), DEFAULT = all grids for hydraulic data, no grids for boundary condition data
4,5	INBRCH(1,I), INGRID(1,I)	2I7	First branch and grid number for input, not needed for hydraulic data
6,7	INBRCH(2,I), INGRID(2,I)	2I7	Second branch and grid number for input, not needed for hydraulic data
8,9	INBRCH(3,I), INGRID(3,I)	2I7	Third branch and grid number for input, not needed for hydraulic data
10			Empty
11,12	INBRCH(4,I), INGRID(4,I)	2I7	Fourth branch and grid number for input, not needed for hydraulic data
.	.	.	.
.	.	.	.
.	.	.	.
3+2*NINGRD(I), 4+2*NINGRD(I)	INBRCH(NINGRD(I),I), INGRID(NINGRD(I),I)	2I7	NINGRD(I) branch and grid number for input, not needed for hydraulic data

**Repeat data set NINPUT times where I = 1 to NINPUT.

Data Set 10 -- TDDS Output

Include only if NOUT > 0

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	OUTTYP(I)	5X,A2	Output data type
2	OUTCON(I)	I7	Number of constituent to be output (1-9, if 10 input 0)
3	OUTBRN(I)	I7	Branch number for output
4	OUTGRD(I)	I7	Grid number for output
5-10			Empty

**Repeat data set NOUT times, I = 1 to NOUT.

Data Set 11 Boundary Conditions

Field	Variable	Format	Description
(Card 1)			
0		10X	Card label
1	NBC	I7	Number of boundary conditions that change during current time step
2-10			Empty
(Card 2)			
0	N,I	2(3X,I2)	Branch N and grid I where boundary condition changes
L	GTRIB(N,L,I)	F7.0	New boundary condition of constituent L at branch N, grid I, L = 1 to NEQ

Repeat card 2 NBC times

Repeat data set 11 for every time step, NHR times

Appendix B

INPUT FILE FORMAT FOR QUAL2.IN

Data set 1-- Universal Coefficients

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Recommended Value</u>	<u>Description</u>
0		10X		Card Label
1	A1	F7.0	3.01	Free convection term in wind function, in mm/day Kpa
2	B1	F7.0	1.13	Mass transfer coefficient in wind function, in mm/(day Kpa(m/s))
3	GROMAX	F7.0	1.0-3.0	Maximum specific growth rate for algae in day ⁻¹
4	CKN	F7.0	0.2-0.4	Nitrogen half-saturation constant for algae in mg/L
5	CKP	F7.0	0.003-0.05	Phosphorus half-saturation constant for algae in mg/L
6	EXCOEF	F7.0		Light extension coefficient for algae in m ⁻¹
7	CKL	F7.0	0.03	Light half-saturation constant for algae growth in Langley minute ⁻¹
8	RESPRT	F7.0	0.05-0.5	Algae respiration rate in day ⁻¹
9-10				Empty

Data Set 2--More Constants

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Recommended Value</u>	<u>Description</u>
0		10X		Card identifier
1	ALPHA1	F7.0	0.08-0.09	Fraction of algae biomass which is nitrogen
2	ALPHA2	F7.0	0.012-0.015	Fraction of algae biomass which is phosphorus
3	ALPHA3	F7.0	1.4-1.8	Oxygen production per unit of algae growth
4	ALPHA4	F7.0	1.6-2.3	Oxygen uptake per unit of algae expired
5	ALPHA5	F7.0	3.0-4.0	Oxygen uptake per unit of ammonia oxidized
6	ALPHA6	F7.0	1.0-1.14	Oxygen uptake per unit of nitrite oxidized
7-10				Empty

Data Set 3--Variable Coefficients

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Recommended Value</u>	<u>Description</u>
			Card 1	
0		10X		Card identifier
1	ALGSET	F7.0	0.2-1.8	Local settling rate for algae in m/day.
2	CKNH3	F7.0	0.1-0.5	Rate constant for biological oxidation of NH ₃ to NO ₂ in day ⁻¹
3	SNH3	F7.0	~	Benthos source rate for ammonia in mg-N day ⁻¹ meter ⁻¹
4	CKNO2	F7.0	0.5-2.0	Rate constant for biological oxidation of NO ₂ to NO ₃ in day ⁻¹ .
5	SPHOS	F7.0	~	Benthos source rate for phosphorus in mg-P day ⁻¹ m ⁻¹ .
6-10				Empty

Data Set 3--Variable Coefficients--Continued

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Recommended Value</u>	<u>Description</u>
			Card 2	
		10X		Card identifier
1	CK1	F7.0	0.1-2.0	Carbonaceous BOD decay rate in day ⁻¹ .
2	CK2	F7.0	0.0-100	Reaeration rate in day ⁻¹ .
3	CK3	F7.0	-0.36-0.36	Carbonaceous sink rate in day ⁻¹ .
4	CK4	F7.0		Benthos consumption of oxygen in mg day ⁻¹ m ⁻¹ .
5	CK5	F7.0	0.5-4.0	Coliform die-off rate in day ⁻¹
6	CK6	F7.0	~	Arbitrary nonconservative decay rate in day ⁻¹ .
7-10				Empty

Repeat Data Set 3 for each reach of each branch starting with branch 1, subreach 1 and ending with branch NBRCH subreach NXSEC(NBRCH)-1.

Data Set 4--Meteorological Variables
(one card for each time step)

<u>Field</u>	<u>Variable</u>	<u>Format</u>	<u>Recommended Value</u>	<u>Description</u>
0		10X		Card identifier
1	TA	F7.0	~	Equilibrium temperature in degree C (air temperature can sometimes be used).
2	V	F7.0	~	Wind speed at in m s ⁻¹ .
3	SONET	F7.0	~	Solar radiation in Langleys (used only to determine algae growth rate).
4-10				Empty

Appendix C

PLOT PROGRAM FOR TIME VARIATION OF CONCENTRATION

A program to plot the time variation of concentration at any point in the network is listed in figure C-1. The program is written to use the DISSPLA¹ software package and is stored in a file called CTPLT.F77. It obtains concentrations from the file PARCEL.OUT assuming data has been stored for every time step. CTPLT.F77 obtains the time step size and network geometry information from the file BLTM.IN.

The program reads BLTM.IN and then queries the user as to which branch contains the desired point, the number of miles the desired point is downstream from the reference point, and the constituent number to be plotted. The reference distance downstream must correspond to the measuring system used to define the location of the grid points in BLTM.IN.

With this information the program reads the file PARCEL.OUT and computes the time variation of concentration at the desired point. The program then displays the maximum concentration, and queries the user for the maximum ordinate desired for the plot (YMAX) and the spacing of the ordinate tick marks (DY). The program then displays the time for the last data point and queries the user for the maximum abscissa for the plot (XMAX) and the spacing of the tick marks (DX) before plotting the graph.

¹The use of Brand names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

Figure C-1.-- Code for program to plot time variation of concentration.

```

C      This program plots concentration vs time and computes the RMS error.
C      CMAX  Maximum computed concentration or max of plot
C      DT    Time step size in hours
C      ER    Error in computed value
C      IP    Code for plotting observed data (1 to plot observed)
C      JTS   Number of time steps from midnight to start of model
C      K     Parcel number
C      L     Constituent number
C      LABEL Name of constituent L
C      LP    Constituent number to be plotted
C      NBRCH Number of branches in model
C      NBRCHP Branch where plot is desired
C      NEQ   Number of equations in model
C      NP    Number of points to be plotted
C      NR    Number of observed concentrations
C      NS    Number of parcels in branch N
C      NXSEC Number of grids in branch N
C      PT(K) Concentration of L in parcel K of branch N
C      PX(K) Grid unit location of u/s boundary of parcel K in branch N
C      RM(I) Miles downstream of grid I in branch N from reference point
C      RMP   Miles downstream where plot is desired
C      SR    Sum of errors
C      SRR   Sum of squares of errors
C      TITLE(20) Title of run
C      X(NP) X plotting position for point NP
C      XMAX  Maximum time plotting position
C      XR(NR) X plotting position for the observer conc point NR
C      YC    Computed value of concentration
C      Y(NP) Y plotting position for point NP
C      YR(NR) Y plotting position for the observer conc point NR
C
C***  BEGIN DIMENSIONING DEFINITION
C
C      NOSC   Maximum number of grids allowed in a branch
C      NOPR   Maximum number of parcels allowed in branch
C      NOCP   Maximum number of computed points to be plotted
C      NOOP   Maximum number of observed points to be plotted
C
C      INTEGER NOSC,NOPR,NOCP,NOOP
C      PARAMETER (NOSC=15,NOPR=150,NOCP=960,NOOP=500)
C
C      + + + LOCAL VARIABLES + + +
C
C      CHARACTER*4 LABEL
C      INTEGER I, IP, J, JTS, K, L, LP, M, N, NBRCH, NBRCHP, NEQI, NN, NR, NS, NXSEC, LUIN
C      #      LUPC, LUOUT, LUDT
C      REAL   AA, CMAX, DT, DX, ER, PT (NOPR) , PX (NOPR) , RM (NOSC) , RMP, SR, SRR,
C      #      TITLE (20) , X (NOCP) , XMAX, XR (NOOP) , YC, Y (NOCP) , YR (NOOP)
C      LUIN=35
C      LUPC=36
C      LUOUT=37
C      LUDT=38
C      OPEN (LUIN, FILE='BLTM.IN')
C      OPEN (LUPC, FILE='PARCEL.OUT')
C      OPEN (LUOUT, FILE='PLT')
C

```

```

C      + + + INPUT FORMATS + + +
C
3500 FORMAT(20A4)
3501 FORMAT(10X,10I7)
3502 FORMAT(10X,10F7.3)
3503 FORMAT(10X,I7,A7,I7)
3504 FORMAT(10X,F7.3,I7)
3600 FORMAT(3I5)
3601 FORMAT(8G10.3)
C
C      + + + OUTPUT FORMATS + + +
C
3700 FORMAT(3G12.4)
3701 FORMAT('Concentration of ',A4,' in branch',I3,'at river mile',
# F7.3)
3702 FORMAT(I5,6F12.2)
3800 FORMAT(2G12.4)
3801 FORMAT(20A4)
WRITE(*,*) 'This program reads PARCEL.OUT, BLTM.IN, and OBS.'
WRITE(*,*) 'It writes the file PLT.'
WRITE(*,*) 'This program is dimensioned for',NOPR, ' Parcels per br
#anch'
WRITE(*,*) '      For',NOSC, ' cross sections per branch.'
WRITE(*,*) '      For',NOCP, ' computed plotting points.'
WRITE(*,*) '      For',NOOP, ' observed plotting points.'
C
C      ***** read data from BLTM.IN *****
C
READ(LUIN,3500) (TITLE(K),K=1,20)
READ(LUIN,3501) NBRCH,I,L,NEQ,JTS
READ(LUIN,3502) DT
WRITE(*,*) 'Constituent number to be plotted = '
READ(*,*) LP
DO 10 L=1,NEQ
  IF (L.EQ.LP) THEN
    READ(LUIN,3503) M,LABEL
  ELSE
    READ(LUIN,3503) M
  END IF
10 CONTINUE
WRITE(*,*) 'Branch number where plot is desired = '
READ(*,*) NBRCHP
DO 20 N=1,NBRCH
  READ(LUIN,3501) NXSEC
  DO 20 I=1,NXSEC
    IF (NBRCHP.EQ.N) THEN
      READ(LUIN,3504) RM(I)
      IF (NEQ.GT.8.AND.I.LT.NXSEC) READ(LUIN,3500) TITLE(20)
    ELSE
      READ(LUIN,3504) XR(I)
      IF (NEQ.GT.8.AND.I.LT.NXSEC) READ(LUIN,3500) TITLE(20)
    END IF
  20 CONTINUE
C

```

```

C ***** READ PLOT DATA *****
C
WRITE(*,*)'River mile of plot = '
READ(*,*) RMP
WRITE(LUOUT,3701) LABEL,NBRCHP,RMP
C
C ***** read PARCEL.OUT and build plot file *****
C
WRITE(LUOUT,*) ' TIME COMPUTED '
NP=0
CMAX=0.0
30 CONTINUE
DO 40 NN=1,NBRCH
READ(LUPC,3600,END=70) J,N,M
IF(N.EQ.NBRCHP) THEN
NS=M
READ(LUPC,3601) (PX(K),K=1,M)
ELSE
READ(LUPC,3601) (XR(K),K=1,M)
END IF
DO 40 L=1,NEQ
IF(L.EQ.LP.AND.N.EQ.NBRCHP) THEN
READ(LUPC,3601) (PT(K),K=1,M)
ELSE
READ(LUPC,3601) (XR(K),K=1,M)
END IF
40 CONTINUE
C WRITE(LUOUT,3600) J,NBRCHP,NS
C WRITE(LUOUT,3601) (PX(K),K=1,NS)
C WRITE(LUOUT,3601) (PT(K),K=1,NS)
M=IFIX(1000.0*RMP)
K=0
50 K=K+1
IF(K.GT.NS) GO TO 60
I=IFIX(PX(K))
AA=PX(K)-FLOAT(I)
AA=RM(I)+AA*(RM(I+1)-RM(I))
NN=IFIX(1000.0*AA)
IF(NN.LE.M) GO TO 50
60 CONTINUE
K=K-1
NP=NP+1
X(NP)=DT*(FLOAT(J+JTS)-0.5)
X(1)=DT*FLOAT(JTS)
IF(X(NP).GT.XMAX) XMAX=X(NP)
Y(NP)=PT(K)
IF(Y(NP).GT.CMAX) CMAX=Y(NP)
WRITE(LUOUT,3700) X(NP),Y(NP)
GO TO 30
70 CONTINUE
C

```

```

C   READ OBSERVED DATA
C
      IP=0
      WRITE(*,*)'Enter 1 to plot observed, n or 0 otherwise '
      READ(*,*,ERR=120)I
      IP=I
      IF(IP.NE.1)GO TO 120
      OPEN(LUOT,FILE='OBS')
      I=0
      READ(LUOT,3801)(TITLE(K),K=1,20)
      WRITE(LUOUT,3801)(TITLE(K),K=1,20)
      READ(LUOT,3801)(TITLE(K),K=1,20)
      WRITE(LUOUT,3801)(TITLE(K),K=1,20)
      WRITE(LUOUT,*)'   TIME      OBSERVED      Error'
80  I=I+1
      READ(LUOT,3800,END=90)XR(I),YR(I)
C   WRITE(LUOUT,3700)XR(I),YR(I)
      IF(XR(I).GT.XMAX) XMAX=XR(I)
      IF(YR(I).GT.CMAX) CMAX=YR(I)
      GO TO 80
90  NR=I-1
C
C   COMPUTE RMS
C
      SR=0.0
      SRR=0.0
      DO 110 I=1,NR
        N=0
100  N=N+1
        IF(N.GT.NP)GO TO 110
        IF(X(N).LE.XR(I)) GO TO 100
        YC=Y(N-1)+(Y(N)-Y(N-1))*(XR(I)-X(N-1))/(X(N)-X(N-1))
        ER=YC-YR(I)
        WRITE(LUOUT,3700)XR(I),YR(I),ER
        SR=SR+ER
        SRR=SRR+ER*ER
110  CONTINUE
      SR=SR/(FLOAT(NR))
      SRR=SRR/(FLOAT(NR))
      WRITE(LUOUT,*)'MEAN ERROR=',SR,' RMS=',SRR,' BASED ON',NR,
# ' POINTS'
C
C   ***** plot results *****
C
120  CONTINUE
C   CALL PTEKAL
      CALL GRPHON
C   CALL HP 7221 (1)
      WRITE(*,*)'The maximum concentration is',CMAX
      WRITE(*,*)'Enter CMAX = '
      READ(*,*) CMAX
      WRITE(*,*)'Enter DY = '
      READ(*,*) DY
      WRITE(*,*)'The maximum time is',XMAX
      WRITE(*,*)'Enter XMAX in hours = '
      READ(*,*)XMAX
      WRITE(*,*)'Enter DX in hours = '
      READ(*,*) DX

```

```
CALL RESET('ALL')
CALL PAGE(11.0,8.5)
CALL AREA2D(10.0,7.0)
CALL XNAME('Time, in hours$',100)
CALL YNAME('Concentration$',100)
CALL GRAF(0.0,DX,XMAX,0.0,DY,CMAX)
CALL CURVE(X,Y,NP,0)
IF(IP.EQ.1)CALL CURVE(XR,YR,NR,-1)
CALL MESSAG('CONSTITUENT $',100,7.0,6.0)
CALL INTNO(LP,'ABUT','ABUT')
CALL ENDPL(0)
CALL DONEPL
CLOSE(LUPC)
CLOSE(LUIN)
ENDFILE(LUOUT)
CLOSE(LUOUT)
IF(IP.EQ.1)CLOSE(LUDT)
STOP
END
```

Appendix D

PLOT PROGRAM FOR CONCENTRATION PROFILES

A program to plot the instantaneous concentration profile in any combination of branches is listed in figure D-1. The program is written for use with the DISSPLA software package and is stored in a file called CXPLT.F77. The program obtains the network geometric information from the file called BLTM.IN and queries the user as to which instantaneous profile is desired from PARCEL.OUT. Recall that instantaneous concentrations for all branches are stored in PARCEL.OUT at a specified time step interval. For example, if data are stored in PARCEL.OUT every 6 time steps and the time step size is one hour, the first set of concentrations in PARCEL.OUT will be at time step 0 (the beginning of the simulation) and the second set of concentrations will be after 6 hours of simulation. So if a concentration profile is desired after 18 hours of simulation, the operator would request the fourth profile in PARCEL.OUT to be plotted. If data were entered every hour, then the nineteenth profile should be requested.

The program then asks for the number of branches to be plotted. Any number of branches can be plotted, and each branch will be plotted in the order that they are input. For example, if branches 1, 3, and 5 were to be plotted with branch 3 on the left, branch 5 on the right, and branch 1 in between, the user would specify 3 branches were to be plotted, and then enter the branch numbers 3, 1, and 5.

The program then sets up the plot file and displays the maximum concentration to be plotted. The user enters the maximum ordinate (YMAX) of the graph and the increments size (DY). The program then displays the maximum abscissa (XMAX) and the increment size (DX) before the graph is plotted.

Figure D-1.-- Code for program to plot concentration profiles.

```

C      THIS PROGRAM PLOTS CONCENTRATION VS DISTANCE
C
C      CMAX      Maximum value of concentration to be plotted
C      DX       X grid spacing on plot
C      DY       Y grid spacing on plot
C      JPO      Number of time steps between output prints for PARCEL.OUT
C      K        Parcel number
C      L        Constituent number
C      LP       Constituent number to be plotted
C      NBP(NBPM) Branches to be plotted
C      NBPM     Number of branches to be plotted
C      NBRCH    Number of branches in model
C      NEQ      Number of equations in model
C      NP       Number of points to be plotted
C      NPN      Output number in file PARCEL.OUT to be plotted
C      NS(N)    Number of parcels in branch N
C      NXSEC(N) Number of grids in branch N
C      PT(N,K)  Concentration of L in parcel K of branch N
C      PX(N,K)  Location of u/s boundary of parcel K in branch N, in grid units
C      RM(N,I)  Miles downstream for grid I in branch N
C      X(NP)    X plotting position for point NP
C      XG(N,I)  Distance of grid I in branch N downstream of origin
C      XS      Maximum distance to be plotted or distance to last point
C      Y(NP)    Y plotting position for point NP
C      TITLE(20) Title of run
C
C*** BEGIN DIMENSIONING DEFINITION
C
C      NOBR     Maximum number of branches allowed in model
C      NOSC     Maximum number of grids allowed in a branch
C      NOPR     Maximum number of parcels allowed in branch
C      NOCP     Twice the maximum number of computed points to be plotted
C
C      INTEGER NOBR,NOSC,NOPR,NOCP
C      PARAMETER (NOBR=10,NOSC=15,NOPR=150,NOCP=560)
C
C      + + + LOCAL VARIABLES + + +C
C
C      INTEGER I, I1, J, JPO, K, L, LP, M, N, NBP (NOBR) , NBRCH, NEQ, NPN,
#      NS (NOBR) , NXSEC (NOBR)
C      REAL    A, CMAX, DX, DY, PT (NOBR, NOPR) , PX (NOBR, NOPR) ,
#      RM (NOBR, NOSC) , X (NOCP) , XG (NOBR, NOSC) , XS, Y (NOCP) , TITLE (20)
C
C      LUIN=35
C      LUPC=36
C      LUOUT=37
C      OPEN (LUIN, FILE='BLTM. IN')
C      OPEN (LUPC, FILE='PARCEL. OUT')
C      OPEN (LUOUT, FILE='PLT')
C

```

```

C      + + + INPUT FORMATS + + +

3500 FORMAT(20A4)
3510 FORMAT(10X,10I7)
3520 FORMAT(10X,10F7.3)
3600 FORMAT(3I5)
3610 FORMAT(8G10.3)
3710 FORMAT(2G12.4)
1001 FORMAT(' Enter title of output (no more than 80 characters)',/)
C
C      + + + OUTPUT FORMATS + + +
C
WRITE(*,*)'This program reads PARCEL.OUT and BLTM.IN.'
WRITE(*,*)'It writes the file PLT.'
WRITE(*,*)'This program is dimensioned for',NOBR, ' branches.'
WRITE(*,*)'      For',NOSC, ' cross sections per branch.'
WRITE(*,*)'      For',NOPR, ' parcels per branch.'
J=NOCP/2
WRITE(*,*)'      For',J, ' plotting points.'

C
C      ***** read data from BLTM.IN *****
C
READ(LUIN,3500)(TITLE(K),K=1,20)
READ(LUIN,3510)NBRCH,I,K,NEQ,J,L,JPO
IF(NBRCH.GT.NOBR)GO TO 9991
READ(LUIN,3520)A
DO 10 L=1,NEQ
  READ(LUIN,3510)M
10 CONTINUE
DO 20 N=1,NBRCH
  READ(LUIN,3510)NXSEC(N)
  I1=NXSEC(N)
  IF(I1.GT.NOSC)GO TO 9992
  DO 20 I=1,I1
    READ(LUIN,3520) RM(N,I)
    IF (NEQ.GT.8.AND.I.LT.I1) READ(LUIN,3500) TITLE(20)
20 CONTINUE

C
C      ***** read plot data *****
C
WRITE(*,*)'Enter time step number of profile to be plotted- '
READ(*,*)NPN
IF(MOD(NPN,JPO).NE.0)WRITE(*,*)'Desired time step not stored'
NPN=1+NPN/JPO
J=(NPN-1)*JPO
WRITE(*,*)'Will plot time step',J
WRITE(*,*)'Enter total number of branches to be plotted- '
READ(*,*) NBPM
DO 30 M=1,NBPM
  WRITE(*,*)'Enter next branch to be plotted- '
  READ(*,*) NBP(M)
30 CONTINUE
WRITE(*,*)'Enter constituent number to be plotted- '
READ(*,*)LP
C

```

```

C      ***** read PARCEL.OUT *****
C
DO 40 I1=1,NPN
  DO 40 M=1,NBRCH
    READ (LUPC,3600) J,N,NS(N)
    IF (NS(N).GT.NOPR) GO TO 9993
    READ (LUPC,3610) (PX(N,K),K=1,NS(N))
    DO 40 L=1,NEQ
      IF (L.EQ.LP) THEN
        READ (LUPC,3610) (PT(N,K),K=1,NS(N))
      ELSE
        READ (LUPC,3610) (X(K),K=1,NS(N))
      END IF
40  CONTINUE
C
C      ***** build plot file *****
C
XS=0.0
DO 60 M=1,NBPM
  N=NBP(M)
  I1=NXSEC(N)
  DO 50 I=1,I1
    XG(N,I)=RM(N,I)-RM(N,1)+XS
50  CONTINUE
  XS=XG(N,I1)
60  CONTINUE
  X(1)=0.0
  Y(1)=0.0
  NP=2
  CMAX=0.0
  DO 80 M=1,NBPM
    N=NBP(M)
    DO 80 K=1,NS(N)
      X(NP)=X(NP-1)
      Y(NP)=PT(N,K)
      NP=NP+1
      IF (NP.GT.NOCP) GO TO 9994
      X(NP)=XG(N,NXSEC(N))
      Y(NP)=PT(N,K)
      IF (CMAX.LT.Y(NP)) CMAX=Y(NP)
      IF (K.EQ.NS(N)) GO TO 70
      I1=IFIX(PX(N,K+1))
      A=PX(N,K+1)-FLOAT(I1)
      X(NP)=XG(N,I1)+A*(XG(N,I1+1)-XG(N,I1))
70  CONTINUE
      NP=NP+1
      IF (NP.GT.NOCP) GO TO 9994
80  CONTINUE
  NP=NP-1
  WRITE(*,1001)
  READ(*,3500) (TITLE(I),I=1,20)
  WRITE(LUOUT,3500) (TITLE(I),I=1,20)
  WRITE(LUOUT,*) '      X      C      PROFILE PLOTTED=',NPN
  DO 90 I=1,NP
    WRITE(LUOUT,3710) X(I),Y(I)
90  CONTINUE
C

```

```

C      ***** plot results *****
C
WRITE(*,*)'the maximum concentration is',CMAX
WRITE(*,*)'enter CMAX'
READ(*,*) CMAX
WRITE(*,*)'enter DY'
READ(*,*) DY
WRITE(*,*)'the maximum distance is',XS
WRITE(*,*)'enter XMAX in miles'
READ(*,*)XS
WRITE(*,*)'enter DX in miles'
READ(*,*) DX
C
CALL PTEKAL
CALL GRPHON
CALL RESET('ALL')
CALL PAGE(11.0,8.5)
CALL AREA2D(10.0,7.0)
CALL XNAME('Distance, in miles$',100)
CALL YNAME('Concentration$',100)
CALL GRAF(0.0,DX,XS,0.0,DY,CMAX)
CALL CURVE(X,Y,NP,0)
NP=1
X(NP)=0.0
Y(NP)=CMAX
DO 100 M=1,NBPM
  NP=NP+1
  IF(NP.GT.NOCP)GO TO 9994
  N=NBP(M)
  X(NP)=XG(N,NXSEC(N))
  Y(NP)=CMAX
  NP=NP+1
  IF(NP.GT.NOCP)GO TO 9994
  X(NP)=X(NP-1)
  Y(NP)=0.0
  NP=NP+1
  IF(NP.GT.NOCP)GO TO 9994
  X(NP)=X(NP-1)
  Y(NP)=CMAX
100 CONTINUE
  NP=NP+1
  IF(NP.GT.NOCP)GO TO 9994
  X(NP)=XS
  Y(NP)=CMAX
  NP=NP+1
  IF(NP.GT.NOCP)GO TO 9994
  X(NP)=XS
  Y(NP)=0.0
  CALL CURVE(X,Y,NP,0)
  CALL MESSAG('CONSTITUENT $',100,7.0,6.0)
  CALL INTNO(LP,'ABUT','ABUT')
  CALL ENDPL(0)
  CALL DONEPL
  GO TO 999
9991 WRITE(*,*)'Too many branches, increase NOBR'
  GO TO 999
9992 WRITE(*,*)'Too many cross sections, increase NOSC'
  GO TO 999
9993 WRITE(*,*)'Too many parcels per branch, increase NOPR'

```

```
GO TO 999
9994 WRITE(*,*) 'Too many plotted points, increase NOCP'
999 CLOSE(LUPC)
CLOSE(LUIN)
ENDFILE(LUOUT)
CLOSE(LUOUT)
STOP
END
```

Appendix E

PLOT PROGRAM FOR HYDRAULIC VARIABLES

A program to plot the time variation of any of the four hydraulic variables at any grid point in the network is listed in figure E-1. The program is written for use with the DISSPLA software package and is stored in a file called FLWPLT.F77. The program obtains the flow data directly from BLTM.FLW and can be used before BLTM.IN is created to check the flow conditions before transport modeling begins. Once the branch number and grid number of the desired plot has been entered by the user, the program queries the user for the time step size and the flow variable to be plotted (discharge, area, top width, or tributary inflow). With this information the program reads the appropriate data from BLTM.FLW and builds the plot file. It then displays the maximum and minimum size of the flow variable to be plotted and request the maximum and minimum ordinates (YMAX,YMIN) for the plot as well as the increment (DY). The program then displays the maximum time to be plotted and request the maximum abscissa of the graph (XMAX) as well as the increment (DX) before plotting the graph. If BLTM.FLW is not used, the TDDS can plot hydraulic data stored in a TDDB.

Figure E-1. -- Code for program to plot time variation of hydraulic data.

```

C      This program builds a file which can be imported to plot flow data.
C      It can also estimate ungaged inflow and plot by use of DISSPLA.
C      FLOW(M)  flow field for M where:
C              M=1  for discharge in cu m/s
C              M=2  for area in sq meters
C              M=3  for top width in meters
C              M=4  for tributary inflow in cu m/s
C      X(NP)  x plotting position for point NP
C      Y(NP)  y plotting position for point NP
C      MP flow number to be plotted
C      NP number of points to be plotted
C      DT time step size in hours
C      NG grid number where flow is desired
C
      INTEGER I, IC, ICT, IENG, II, IIT, IO, K, J, LUIN, LUOBS, LUOUT, M, MP,
#         N, NB, NG, NP
      REAL   A1, A2, BLK(20), C, DST, DT, DX, DY, ER, FLOW(4), Q, QMAX, QMIN, SR,
#         SRR, T, TT, XC, X(2000), XMAX, XO(500), Y(2000), YC, YMAX, YMIN,
#         YO(500)
      LUIN=35
      LUOUT=36
      LUOBS=37
      OPEN(LUIN, FILE='BLTM.FLW')
      OPEN(LUOUT, FILE='PLT')
C
C          + + + FORMATS + + +
C
1500 FORMAT(I5, I5, I5, 4E18.5)
1600 FORMAT('Flow in branch', I3, ' grid', I3, ' DT=', F7.3)
1601 FORMAT('Area in branch', I3, ' subreach', I3, ' DT=', F7.3)
1602 FORMAT('Top width in branch', I3, ' subreach', I3, ' DT=', F7.3)
1603 FORMAT('Tributary inflow to branch', I3, ' grid', I3, ' DT=', F7.3)
1604 FORMAT(4G12.4)
1700 FORMAT(20A4)
C
C      ***** read plot data *****
C
      WRITE(*,*) 'enter branch number where plot is desired  '
      READ(*,*) NB
      WRITE(*,*) 'enter grid number where plot is desired  '
      READ(*,*) NG
      WRITE(*,*) 'enter time step size, in hours  '
      READ(*,*) DT
      WRITE(*,*) 'enter 1 to plot discharge at grid'
      WRITE(*,*) 'enter 2 to plot cross sectional area in subreach'
      WRITE(*,*) 'enter 3 to plot top width in subreach'
      WRITE(*,*) 'enter 4 to plot tributary inflow at grid  '
      READ(*,*) MP
      WRITE(*,*) 'enter 1 for English units, 0 for metric.  '
      READ(*,*) IENG
      IF(MP.EQ.1) WRITE(LUOUT, 1600) NB, NG, DT
      IF(MP.EQ.2) WRITE(LUOUT, 1601) NB, NG, DT
      IF(MP.EQ.3) WRITE(LUOUT, 1602) NB, NG, DT
      IF(MP.EQ.4) WRITE(LUOUT, 1603) NB, NG, DT
      WRITE(LUOUT, *) '   Time   Computed'
      NP=0
      X(1)=0.0
      IC=0

```

```

1 CONTINUE
  READ (LUIN,1500,END=2) J,N,I,(FLOW(M),M=1,4)
  IF (N.NE.NB) GO TO 1
  IF (I.NE.NG) GO TO 1
  IF (IC.EQ.0) QMAX=FLOW(MP)
  IF (IC.EQ.0) QMIN=FLOW(MP)
  IC=1
  NP=NP+1
  IF (NP.GT.1) X(NP)=DT*(FLOAT(NP)-1.5)
  Y(NP)=FLOW(MP)
  IF (QMAX.LT.Y(NP)) QMAX=Y(NP)
  IF (QMIN.GT.Y(NP)) QMIN=Y(NP)
  WRITE (LUOUT,1604) X(NP),Y(NP)
  GO TO 1
2 CONTINUE
C
C   BUILD OBSERVED FLOW FILE
C
  IC=0
  WRITE(*,*) 'Enter 1 to plot observed, q otherwise '
  READ(*,*,ERR=3) ICT
  IC=ICT
3 IF (IC.NE.1) GO TO 10
  OPEN (LUOBS,FILE='OBS')
  IO=0
  II=0
  WRITE(*,*) 'Enter 1 to estimate ungaged inflow, q otherwise '
  READ(*,*,ERR=11) IIT
  II=IIT
  WRITE(*,*) 'Enter distance upstream to ungaged inflow (miles) '
  READ(*,*) DST
  WRITE(*,*) 'Enter A1 '
  READ(*,*) A1
  WRITE(*,*) 'Enter A2 '
  READ(*,*) A2
11 READ (LUOBS,1700) (BLK(K),K=1,20)
  WRITE (LUOUT,1700) (BLK(K),K=1,20)
  READ (LUOBS,1700) (BLK(K),K=1,20)
  WRITE (LUOUT,1700) (BLK(K),K=1,20)
  IF (II.NE.1) WRITE (LUOUT,*) '   Time      Flow Obs      error'
  IF (II.EQ.1) WRITE (LUOUT,*) ' Time in      ungaged      Flow Obs      Time
# Obs'
12 READ (LUOBS,1604,END=13) XC,Q
  IO=IO+1
  XO(IO)=XC
  YO(IO)=Q
  GO TO 12
13 CONTINUE
C
C   COMPUTE RMS
C
  SR=0.0
  SRR=0.0
  DO 16 I=1,IO
    N=1
14 N=N+1
  IF (X(N).LT.XO(I)) GO TO 14
  YC=Y(N-1)+(Y(N)-Y(N-1))*(XO(I)-X(N-1))/(X(N)-X(N-1))

```

```

ER=YO(I)-YC
IF(II.EQ.0) THEN
  WRITE(LUOUT,1604) XO(I), YO(I), ER
ELSE
  C=(YO(I)**(1.0-A2))/(A1*A2)
  IF(IEING.EQ.0) C=C/0.3048
  TT=DST*5280.0/(C*3600.0)
  T=XO(I)-TT
  WRITE(LUOUT,1604) T, ER, YO(I), XO(I)
END IF
SR=SR+ER
SRR=SRR+ER*ER
16 CONTINUE
SR=SR/(FLOAT(IO))
SRR=SRR/(FLOAT(IO))
WRITE(LUOUT,*) 'Mean Error=', SR, ' RMS=', SRR, ' based on', IO, ' Points
#'
10 CONTINUE
C
C ***** plot results *****
C
C CALL HP 7475 (1)
C CALL HP7475
C CALL TK41(4105) "4105 is the number on the tecktronics machine"
C CALL PTEKAL
C CALL GRPHON
WRITE(*,*) 'the maximum computed flow is', QMAX
WRITE(*,*) 'enter YMAX '
READ(*,*) YMAX
WRITE(*,*) 'the minimum computed flow is', QMIN
WRITE(*,*) 'enter YMIN '
READ(*,*) YMIN
YC=ABS(YMIN)
IF(YC.LT.0.00001) YMIN=0.0000001
WRITE(*,*) 'enter DY '
READ(*,*) DY
WRITE(*,*) 'the maximum time is', X(NP)
WRITE(*,*) 'enter XMAX in hours '
READ(*,*) XMAX
WRITE(*,*) 'enter DX in hours '
READ(*,*) DX
CALL RESET('ALL')
CALL PAGE(11.0,8.5)
CALL AREA2D(10.0,7.0)
CALL XNAME('Time, in hours$',100)
IF(IEING.EQ.1) GO TO 21
IF(MP.EQ.1) CALL YNAME('Discharge, in cu m/s$',100)
IF(MP.EQ.2) CALL YNAME('Area, in sq meters$',100)
IF(MP.EQ.3) CALL YNAME('Top width, in meters$',100)
IF(MP.EQ.4) CALL YNAME('Tributary discharge, in cu m/s$',100)
GO TO 22
21 CONTINUE
IF(MP.EQ.1) CALL YNAME('Discharge, in cu ft/s$',100)
IF(MP.EQ.2) CALL YNAME('Area, in sq feet$',100)
IF(MP.EQ.3) CALL YNAME('Top Width, in feet$',100)
IF(MP.EQ.4) CALL YNAME('Tributary discharge, in cu ft/s$',100)
22 CONTINUE
CALL GRAF(0.0,DX,XMAX,YMIN,DY,YMAX)

```

```
CALL CURVE (X, Y, NP, 0)
IF (IC.EQ.1) CALL CURVE (XO, YO, IO, -1)
CALL MESSAG ('GRID $', 100, 7.0, 6.0)
CALL INTNO (NG, 'ABUT', 'ABUT')
CALL ENDPL (0)
CALL DONEPL
CLOSE (LUIN)
ENDFILE (LUOUT)
CLOSE (LUOUT)
IF (IC.EQ.1) CLOSE (LUOBS)
STOP
END
```

Appendix F

USE OF TIME-DEPENDENT DATA SYSTEM WITH BLTM

A Time-Dependent Data System (TDDS) has been developed by Regan (written communication, 1986) for the U.S. Geological Survey's BRANCH unsteady flow model (Schaffranek and others, 1981). The TDDS is a useful tool for handling large amounts of time-dependent data that, for example, may be needed in a BLTM simulation with several constituents. Data is stored in a direct access file by the TDDS for specific data types, grid points, and times. The TDDS allows the user to read data from several different sources and also to summarize, delete, print, plot, and modify the data.

A TDDS interface subroutine links the BLTM to the TDDS. This subroutine is very similar to the subroutine that links the Lagrangian Transport Model for rivers to the TDDS (Schoellhamer and Jobson, 1986a, 1986b). Either the flow field (discharge, area, top width, and tributary inflow) or flow field and boundary conditions (upstream concentration, inflow concentrations, and meteorological conditions) can be read from the TDDS. BLTM grid point concentration output can also be stored with the TDDS.

First, the user must select the scope of the TDDS data management with the input variable ITDDS. Then the number of data types to be input, the number of time series to be output, and the value of the TDDS variable LIST is read by the TDDS interface subroutine. The beginning and ending times of the simulation (year, month, day, hour, and minute) and the TDDS station identification number for each BLTM grid point must be provided. Each data type to be input must be specified along with the number of readings per day that are stored in the TDDS, number of grid points at which input is needed (tributary discharge and boundary condition data types only), and the BLTM branch and grid point numbers (tributary discharge and boundary condition data types only). The available data types and their units are listed in Table F-1. Data is read from the TDDS every ten BLTM simulation time steps to optimize both core storage and I/O requirements. The beginning and ending times of each data acquisition are calculated, the data is retrieved, and this data is converted by linear interpolation from the TDDS time step to the BLTM time step. The only compatibility requirement of the two time steps is that a TDDS data point must fall on every tenth (0, 10, 20, ...) BLTM time step. Figure F-1, which is a chart of common time steps and their compatibility, shows that this is not a severe restriction if both data sets start at the same time (time step zero). Each time series to be output must be specified with a data set type, constituent number, branch number, and grid point number. The time series to be stored with the TDDS are stored in an array until the end of the simulation when they are stored with the TDDS.

Table F-1.--Time-Dependent Data System data types

Name	Data Type
> A<	Cross-sectional area [square feet or meters]
AP	Atmospheric pressure [kilopascals]
AT	Atmospheric temperature [Celsius]
> B<	Top width [feet or meters]
C#	Concentration of constituent #, where #=1 to NEQ (10=0)
M#	Measured river concentration of constituent #, where #=1 to NEQ (10=0)
> Q<	Flow rate [cubic feet or meters per second]
>QT<	Tributary flow rate [cubic feet or meters per second]
RA	Incoming atmospheric radiation [cal per sq cm per hour]
RS	Incoming solar radiation [cal per sq cm per hour]
T#	Concentration of constituent # for tributary inflows, where #=1 to NEQ (10=0)
WS	Wind speed [meters per second]

**NOTE: >DATA TYPE< denotes hydraulic data, all other data types are boundary condition data.

		Time-Dependent Data System Time Step, in minutes						
		1	5	6	10	15	30	60
Branched Lagrangian Transport Model Time Step, in minutes	1	X	X		X			
	5	X	X		X			
	6	X	X	X	X	X	X	X
	10	X	X		X			
	15	X	X	X	X	X	X	
	30	X	X	X	X	X	X	X
	60	X	X	X	X	X	X	X
	X Compatible Time Steps							

Figure F-1.--Branch Lagrangian Transport Model/Time-Dependent Data System Compatible Time Steps for the Same Initial Time