

USERS MANUAL FOR A ONE-DIMENSIONAL
LAGRANGIAN TRANSPORT MODEL

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CONVERSION FACTORS

The Lagrangian Transport Model is capable of receiving input in either English or Metric (SI) 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</u>	<u>BY</u>	<u>TO OBTAIN</u>
feet	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)	1.609	kilometers per hour (km/hr)
square feet per second (ft ² /s)	0.0929	square meters per second (m ² /s)
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: °F = 1.8°C + 32
 °C = (°F - 32)/1.8

USERS MANUAL FOR A ONE-DIMENSIONAL

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ABSTRACT

A one-dimensional Lagrangian transport model for simulating water-quality constituents such as temperature, dissolved oxygen, and suspended sediment in rivers is presented in this Users Manual. One-dimensional transport modeling theory and capabilities, restrictions, techniques, and optional capabilities of the model are briefly presented and the application of the model is thoroughly discussed. Appendices present input and output file formats and three example applications.

INTRODUCTION

A one-dimensional transport model can be a useful tool for predicting the fate of water-quality constituents in rivers. Such a model simulates the longitudinal movement of constituents as they are transported downstream. Direct modeling of secondary currents, stratification, transverse mixing, and other multi-dimensional phenomena are excluded. For example, the effect of a power plant discharge on water temperature is modeled by assuming that the outflow immediately mixes uniformly across the river cross section and is transported by the cross-sectionally averaged flow velocity. The primary factor in transport modeling is the flow of the river, called convection, which moves the constituents downstream. As convection occurs, the constituents tend to disperse in the longitudinal direction. Other factors may include the mixing of both point and non-point sources and the decay of constituents with time.

Simulation of these processes is accomplished by solving the convection-dispersion equation. This equation is derived by considering the principle of conservation of mass and must be solved by numerical approximation. Most solution techniques use an Eulerian reference frame that fixes the computational nodes in space. Although Eulerian modeling is easy to conceptualize, the computations are fairly difficult and the results can be inaccurate, oscillatory, and unstable. The alternative is a Lagrangian reference frame which eliminates many of the Eulerian difficulties.

Lagrangian transport modeling moves the computational nodes, which are in reality parcels of water, with the flow of the river. Even though the tracking of parcels requires much bookkeeping, the troublesome convection term is eliminated from the convection-dispersion equation. As parcels pass both point and non-point sources, the inflow is mixed and new parcel

concentrations are computed. In addition, decay is computed within each parcel during each simulation time step.

A one-dimensional Lagrangian transport model, called the LTM, for simulating water-quality constituents such as temperature, dissolved oxygen, and suspended sediment in rivers is presented in this Users Manual. One-dimensional transport modeling theory and Lagrangian modeling techniques are briefly presented and the application of the model is thoroughly discussed. A companion document serves as a Programmers Manual for the LTM (Schoellhamer and Jobson, 1986). The Programmers Manual describes how the LTM works in detail and lists program codes.

The LTM can simulate both steady and unsteady streamflow in addition to variable boundary conditions and solute loads. Time-dependent data can be input from the data base of the Time-Dependent Data System (TDDS, Krug and others, written commun., 1983). Input may be in either English or metric units. Output options include storing output either with the TDDS or in direct access files, calculating a root-mean-squared error, calling a user-written plotting subroutine, and writing decay coefficients. The output includes grid concentration, initial parcel concentration, travel time, and change in concentration due to decay, dispersion, lateral inflows, and tributary inflows.

Decay and constituent reactions are modeled by determining decay coefficients in a subroutine that may be written by the user to suit his particular needs. Examples of three different decay-coefficient subroutines are presented in this Users Manual and listed in the LTM Programmers Manual (Schoellhamer and Jobson, 1986). One of these subroutines uses the reaction kinetics of the QUAL II water-quality model (Roesner and others, 1977a, 1977b), thus providing the advantages of unsteady Lagrangian calculations and the QUAL II reaction kinetics. The user, however, should not use any of the example kinetics if they do not apply to his particular problem. The LTM Programmers Manual (Schoellhamer and Jobson, 1986) describes how to write a decay-coefficient subroutine if the existing routines are not satisfactory.

This Users Manual describes one-dimensional transport theory, the LTM, and how to apply the model. Appendices A thru E list input file formats. Appendices F, G, and H contain example applications of the LTM.

ONE-DIMENSIONAL TRANSPORT THEORY

The convection-dispersion equation first will be derived for a conservative substance in the Eulerian reference frame and then the Lagrangian equivalent will be presented. The Eulerian reference frame is stationary while the Lagrangian reference frame moves with the river flow. For example, an observer standing on a bridge views a river from the Eulerian reference frame while an observer in a drifting boat views the

river from the Lagrangian reference frame. After the equations are derived, the solution techniques for the convection-dispersion equation will be discussed.

Derivation of the Convection-Dispersion Equation

Figure 1 shows a non-moving (Eulerian) incremental control volume of cross-sectional area, Δa , and incremental longitudinal length, Δx . U is the mean cross-sectional velocity and u is the local deviation from U . Thus the conservation of mass, which states that the accumulation of mass in the incremental control volume equals the difference between the mass entering and the mass leaving, gives

$$\frac{\partial(c \Delta x \, da)}{\partial t} = c(U + u) \, da - \left[c(U + u) \, da + \frac{\partial(c(U + u)da)}{\partial x} \Delta x \right] \quad (1)$$

in which c is the concentration of the transported constituent, t is time, and the incremental cross-sectional area is written with the differential expression da . Equation 1 neglects molecular and turbulent diffusion which are usually small relative to differential convection. Simplification gives

$$\frac{\partial(c \, da)}{\partial t} = -\frac{\partial(c(U + u)da)}{\partial x} \quad (2)$$

Integration over the entire cross-sectional area yields

$$\frac{\partial}{\partial t} \int^A c \, da = -\frac{\partial}{\partial x} \int^A c \, U \, da - \frac{\partial}{\partial x} \int^A c \, u \, da \quad (3)$$

Evaluating the first two integrals and noting that U is not a function of da , one derives the transport equation for the cross section

$$\frac{\partial AC}{\partial t} = -\frac{\partial AUC}{\partial x} - \frac{\partial}{\partial x} \int^A c \, u \, da \quad (4)$$

in which C is the average cross-sectional concentration and A is the cross-sectional area. Application of the differentiation product rule produces

$$C \frac{\partial A}{\partial t} + A \frac{\partial C}{\partial t} = -C \frac{\partial AU}{\partial x} - A U \frac{\partial C}{\partial x} - \frac{\partial}{\partial x} \int^A c \, u \, da \quad (5)$$

Equation 5 can be simplified with the continuity equation for the control volume, which is

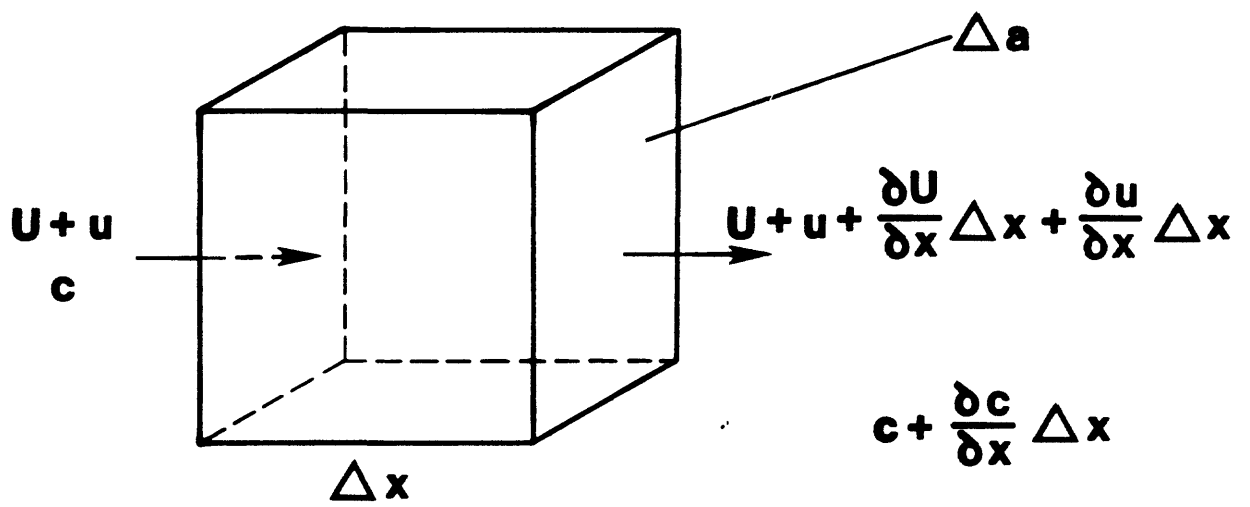


Figure 1.--Incremental control volume.

$$\frac{\partial(\Delta x \, da)}{\partial t} = (U + u) \, da - \left[(U + u) \, da + \frac{\partial}{\partial x} ((U + u)da)\Delta x \right] \quad (6)$$

Simplification, integration over the cross-sectional area, and the fact that the integral of u over the cross-sectional area is zero gives

$$\frac{\partial A}{\partial t} = - \frac{\partial AU}{\partial x} \quad (7)$$

Substitution of equation 7 into equation 5 and simplification gives

$$A \frac{\partial C}{\partial t} = - AU \frac{\partial C}{\partial x} - \frac{\partial}{\partial x} \int^A c \, u \, da \quad (8)$$

The integral in equation 8 is the dispersion term. This term primarily accounts for the reduction of a three-dimensional phenomenon to one dimension. The integral is approximated with the Boussinesq assumption wherein the local deviation from the mean velocity is considered analogous to a turbulent velocity fluctuation such that

$$\frac{1}{A} \int^A u \, c \, da = -D_x \frac{\partial C}{\partial x} \quad (9)$$

where D_x is the longitudinal dispersion coefficient. Finally, equation 9 is substituted into equation 8 and A is assumed to be independent of x . This assumption is relatively minor by comparison with the Boussinesq assumption. The result is

$$\frac{\partial C}{\partial t} = -U \frac{\partial C}{\partial x} + \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) \quad (10)$$

Equation 10 is the Eulerian one-dimensional transport equation for a conservative substance, also called the convection-dispersion equation. The first term on the right hand side is the convective term which accounts for the downstream movement of mass in the river. This term is the most troublesome term for nonanalytical numerical solutions of the transport equation because it can cause numerical dispersion, overshoot, undershoot, negative concentrations, oscillations, and instabilities (Cunge, and others, 1980, Gray and Pinder, 1976, Grenney and others, 1978, Gresho and Lee, 1981, Jobson, 1980, Sobey, 1984, van Genuchten and Gray, 1978, and Varoglu and Finn, 1978). The second term is the dispersion term which accounts for the reduction of a three-dimensional problem to one dimension (Jobson, 1981).

The Lagrangian one-dimensional transport equation is derived similarly with the important exception that the incremental control volume is assumed

to be moving at the mean cross-sectional velocity U . Thus the Lagrangian equivalent of equation 10 is found by setting U equal to zero in equation 1. The derivation is then identical to the Eulerian derivation. The resulting one-dimensional Lagrangian transport equation for a conservative substance is

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) \quad (11)$$

Equation 11 is identical to equation 10 with the exception that the troublesome convective term is eliminated.

Solution Techniques For the Convection-Dispersion Equation

With the one-dimensional transport equation developed, a solution technique has to be chosen. Due to the complexity of both the Eulerian and Lagrangian forms of the equation, an exact solution is not available for natural rivers so a numerical approximation must be developed. The three principal factors that contribute to all numerical solution techniques are the reference frame, the order of continuity enforced in the system, and the source of the flow field.

Transport problems are most commonly solved within an Eulerian reference frame because it is relatively convenient. The river is discretized by grid points at which equation 10 is solved. But, as previously mentioned, the troublesome convective term in the Eulerian transport equation can cause inaccuracies, oscillations, and instabilities. These problems are reduced by complex solution schemes (Holly and Preissmann, 1977, and Pinder and Shapiro, 1979) that have relatively high computational costs.

Combined Eulerian-Lagrangian methods (ELM, also called moving coordinate systems) have recently been developed in an effort to eliminate these problems in both one and two dimensions (Casulli, 1985, Cheng and others, 1984, Douglas and Russell, 1982, Holly and Usseglio-Polatera, 1984, Neumann, 1981, O'Neill, 1981, Sobey, 1983, Thomson and others, 1984, Varoglu and Finn, 1978, and Varoglu and Finn, 1980). Basically, for every time step and grid point, the ELM uses the flow field to determine the initial location of the particle that will conclude the present time step at a grid point. The concentration at this initial particle location is determined by interpolation from the Eulerian grid values, thus solving the convection term. The change in concentration of this particle due to dispersion is calculated using either an Eulerian or a Lagrangian reference frame. The basic disadvantage of the ELM is that the pure Lagrangian transport equation is not fully utilized because particle concentrations must be interpolated with higher order schemes that, although an improvement, are still susceptible to Eulerian numerical difficulties (Casulli, 1985).

A pure Lagrangian reference frame tracks particles or 'parcels' of water by moving them with the flow field. This is identical to the control volume movement used to derive the Lagrangian transport equation. Elimination of the convective term without the need for interpolation outweighs the disadvantage of increased bookkeeping needed to track the parcels (Jobson, 1980). In addition, parcel tracking can be eliminated for steady nonuniform flows (McBride and Rutherford, 1984).

The second factor that contributes to the numerical solution of the transport equation is the order of continuity of the concentration enforced in the system. As shown in Figure 2, no continuity means that discontinuities exist in the longitudinal concentration profile, zero order continuity enforces continuity of concentration, and first order enforces continuity of the first derivative (slope) of concentration. Sobey (1984) shows that higher order solution schemes can improve Eulerian solutions and that a zero order Lagrangian scheme (Sobey's 1983 fractional step algorithm or FSA) is more accurate than a first order Eulerian scheme. But for Lagrangian schemes Schoellhamer (1985) shows that non-enforcement of continuity (as used in the LTM) is almost as accurate as zero order continuity (i.e. the FSA). Thus the selection of a Lagrangian reference frame is more important than the use of higher order continuity and the most cost-effective solution appears to be a noncontinuous Lagrangian scheme.

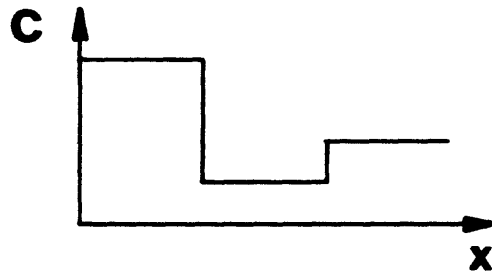
The third primary factor in developing a numerical solution is the source of the flow field. The flow field is either solved simultaneously with the transport equation or it is solved separately and input to the flow model. The advantage of solving the flow and transport equations in tandem is that any interactions between flow and concentration (as with highly concentrated sediment flows) can be modeled. The disadvantage is that if the hydraulics and transport are independent, as is usually the case, the same flow field must be re-solved for each desired solution of the transport equation. Separate solution of the system hydraulics and transport allows one flow field to be used for as many transport solutions as needed to calibrate a transport model.

The most desirable factors to incorporate into a one-dimensional transport model are a Lagrangian reference frame combined with non-enforcement of nodal continuity and an externally solved flow field. The Lagrangian Transport Model has these key attributes.

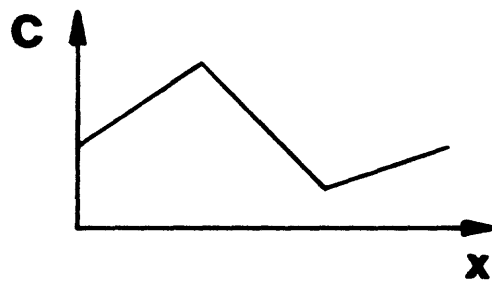
THE LAGRANGIAN TRANSPORT MODEL

The capabilities and restrictions of the LTM will be presented and the techniques used by the model to simulate physical processes will be discussed briefly. These techniques are presented more completely in the LTM Programmers Manual (Schoellhamer and Jobson, 1986). The optional capabilities of the LTM are also discussed.

NO CONTINUITY



ZERO ORDER CONTINUITY



FIRST ORDER CONTINUITY

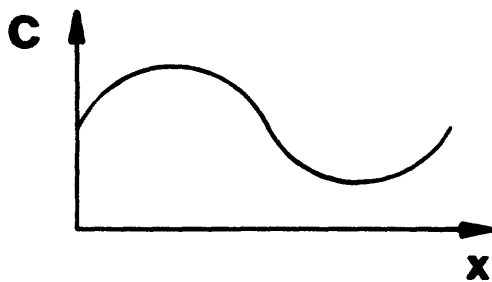


Figure 2.--Nodal continuity.

Capabilities and Restrictions

The LTM can model the longitudinal movement and fate of up to ten water-quality constituents in a riverine environment. The restrictions of the model include one-dimensionality, unidirectional flow, and fixed channel geometry. The LTM does not perform hydraulic calculations. The flow field at fixed grid points, including discharge, cross-sectional area, and possibly top width, must be provided by the user. The flow can either be constant with time (steady) or vary with time (unsteady). The physical processes of dispersion and decay are simulated by the LTM. The effect of tributaries and lateral inflows can also be simulated.

The user can define the constituents and the constituents' reaction kinetics by writing the necessary FORTRAN computer code in a subroutine. Instructions on how to write the decay-coefficient subroutine are given in the LTM Programmers Manual. Preparation of this subroutine is not difficult and may be necessary depending upon the specific needs of the user. This document presents three different sets of reaction kinetics in the Appendices for a conservative constituent model, a four constituent oxygen model, and a ten constituent water-quality model that uses the reaction kinetics of the QUAL II water-quality model. This hybrid LTM/QUAL II model can mimic the QUAL II model results and provide the significant benefit of Lagrangian calculations (Schoellhamer, in press).

Techniques

The five physical process that are directly modeled by the LTM are convection, dispersion, constituent decay, tributary or point source mixing, and lateral inflow mixing. The modeling techniques used by the LTM are outlined here and presented in detail in the LTM Programmers Manual (Schoellhamer and Jobson, 1986).

Convection is the movement of water-quality constituents with the river flow. For example, when dye is dumped in a river the dye will move downstream. The LTM computes convection by tracking the movement of parcels of water that are identical to the control volumes previously introduced. The river reach being modeled may contain from a few to several hundred parcels, each with a known volume of water and known concentrations of each constituent. Lagrangian calculations are performed by moving each parcel at the average flow velocity of the river reach containing the parcel. The user discretizes the river with non-uniformly spaced fixed (Eulerian) grid points at which the flow field (steady or unsteady) is provided to the LTM. Thus the user has the convenience of defining the system in a Eulerian reference frame and the advantage of Lagrangian calculations. The concentration of every constituent is specified at the upstream boundary where a new parcel is introduced every time step. Therefore the chosen simulation time step controls the number of computational elements (parcels) and thus the accuracy of the solution. All other parcels are moved a

distance downstream that depends on the flow velocity and simulation time step. Parcels are numbered from the upstream boundary in ascending order and each parcel contains a volume of water that is changed only when the parcel passes either a point or a non-point source or sink of water. The change in parcel concentrations due to dispersion, decay, tributary inflows, and lateral inflows is also tracked.

As a slug of dye moves downstream it will spread out in the longitudinal direction because of dispersion. Dispersion is calculated by the LTM based on an exchange flow between neighboring parcels. The boundary between neighboring parcels is moved at the mean flow velocity, but in reality a velocity profile exists at the boundary so water near the bed is moving slower than water near the surface as shown in Figure 3. Faster moving water that flows from a parcel into its adjacent downstream parcel is replaced with slower moving water from that adjacent parcel. The parcel volumes do not change, but each parcel has inflows from and discharges to its two neighboring parcels. The inter-parcel discharge is a user-defined fraction of the river discharge. Schoellhamer and Jobson (1986) show that for steady flow

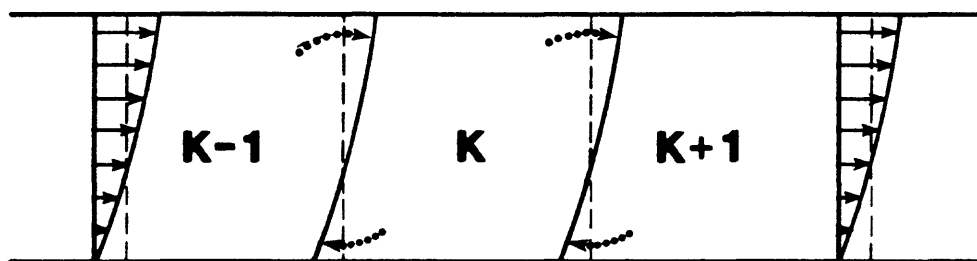
$$DQQ = \frac{D_x}{U^2 \Delta t} \quad (12)$$

where DQQ is the ratio of inter-parcel discharge to river discharge and Δt is the simulation time step. The change in parcel concentrations due to dispersion are calculated with a basic mixing equation. Instabilities could result if the exchanged volume is greater than or equal to half the parcel volume so the simulation time step is subdivided if needed to insure unconditional stability.

Constituents may react with each other, grow, or decay. For each constituent modeled, the decay in each parcel during each time step is

$$\Delta C_L = [S_L + \sum_{\ell=1}^N XK_{L,\ell} (C_\ell - CR_{L,\ell})] \Delta t \quad (13)$$

where L is the constituent number, ℓ is a counter, N is the total number of constituents modeled, XK is an exchange coefficient, CR is an equilibrium concentration, and S is a source flux of constituent L. The coefficients XK, CR, and S are calculated in the decay-coefficient subroutine and they can be functions of any LTM variable or of any value read from a file. Thus the user can easily define the reaction kinetics that best simulate the actual physical system being modeled. Readers should refer to the LTM Programmers Manual if they are interested in defining their own reaction



EXPLANATION

→ **x**



VELOCITY PROFILE



PARCEL BOUNDARY



INTER-PARCEL FLOW

Figure 3.--Inter-parcel flows.

kinetics. This Users Manual presents examples of the three different sets of reaction kinetics that are provided with the model.

The effect of both tributaries (point sources) and lateral inflows on the river can also be modeled. The user must provide both discharges (steady or unsteady) and concentrations of these inflows. Point and nonpoint withdrawals can also be simulated by specifying a negative inflow. Inflows are mixed with a basic mixing equation. Point sources must be located at a grid point used to define the flow field and lateral inflows must be inclusively located between two grid points. Dispersion upstream from either a point source or the upstream boundary of a lateral inflow is not permitted in order to prevent the effect of the inflow from propagating upstream. In addition, point sources are assumed to be located just downstream from a grid point and the upstream boundary of a lateral inflow is also located just downstream from a grid point so neither has an effect at the grid point where their location is specified.

Optional Capabilities

The optional capabilities available within the LTM include input in either English or metric units, simulation in steady or unsteady flow, use of a time-dependent data system for data management, root-mean-squared error calculation, storage of results in direct access files, a call to a user-written subroutine PLOT for additional output, and printing of the decay coefficients.

The input data is read in the unit system selected by the input variable METRIC. If English units are used the unit of length is feet (cubic feet per second, square feet, etc.) except for the locations of grid points which are in river miles. If metric units are used the unit of length is meters (cubic meters per second, square meters, etc.) except for the locations of grid points which are in river kilometers. The program performs calculations with metric units so the initial conditions are always listed in metric units.

The steady/unsteady option is chosen with the input variable IUNSTD. For steady flow, the discharge at the upstream boundary (grid number one), point and non-point inflows, cross-sectional areas, and top widths are read at the beginning of the simulation. Average velocities at grids and in reaches are calculated from the input values and all of this hydraulic data is used throughout the simulation. Note that, even though the hydraulics are steady, meteorological conditions, upstream concentration, and inflow concentrations can change at every time step.

For simulation of transport in unsteady flow, the flow field must be read from an external source because the LTM does not compute the flow field. Either of two sources can be used, the external file UNSTEADY.DATA or a time-dependent data system. The file UNSTEADY.DATA contains the flow

field information at every grid point at the end of every time step (including the initial conditions at time step zero). The flow field information is velocity, cross-sectional area, top width, point source inflow just downstream from each grid point, and lateral inflow in the reach downstream from each grid point. The specific file format is given in Appendix C. All values should be for a particular grid point at the end of a particular time step because the program computes reach and time averaged values.

A Time-Dependent Data System (TDDS) has been developed by Krug and others (written commun., 1983) 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 an unsteady simulation with several constituents. Data is stored in a direct access file by the TDDS for specific data types, grid points, and times. With the TDDS, data can be read from several different sources, summarized, deleted, printed, plotted, and modified.

A TDDS interface subroutine links the LTM to the TDDS (Schoellhamer and Jobson, 1986). Either the flow field (discharge, area, top width, tributary inflow, and lateral inflow), boundary conditions (upstream concentration, inflow concentrations, meteorological conditions, and measured river concentrations for the error calculation), or both can be read from the TDDS. Output can also be stored with the TDDS.

First, the user must select the scope of the TDDS data management with the input variable IUNSTD. Then the number of data types to be input and 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 LTM grid point must be provided. In addition, each data type to be input/output must be specified along with the readings per day (input only), number of grids at which input/output is needed, and the LTM grid numbers. The available data types and their units are listed in Table 1. Data is read from the TDDS every ten LTM 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 LTM 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, ...) LTM time step. Figure 4, 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). Finally, the desired output values, which are temporarily stored in file GRID.DATA (described shortly), are sent to the TDDS at the end of the simulation.

To expedite model calibration, an optional root-mean-squared (RMS) error calculation is included in the LTM. The simulation concentrations are compared to measured concentrations and the RMS error is

Name	Data Type
> A<	Cross-sectional area [square feet or meters]
AP	Atmospheric pressure [kilopascals]
AT	Atmospheric temperature [Celcius]
> B<	Top width [feet or meters]
C#	Concentration of constituent #, where #=1 to NEQ (10=0)
L#	Concentration of constituent # of lateral inflows, 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]
>QL<	Lateral flow rate [square 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.

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

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

Figure 4.--Lagrangian Transport Model/Time-Dependent Data System Compatible Time Steps For the Same Initial Time

$$\sqrt{\frac{1}{n} \sum_{\ell=1}^n (GT_{\ell} - TACT_{\ell})^2} \quad (14)$$

where GT is a computed grid concentration, TACT is an actual concentration, and n is the number of RMS calculations made. If the actual concentration is less than zero, then no RMS calculation is performed for that data point.

The variable IRMS controls whether an RMS calculation will be performed, the time interval at which the error is calculated, and the source of the actual values, either the external file TOBS.INPUT or the TDDS. The error will be calculated every |IRMS| time steps, so if |IRMS| is one the RMS error will be calculated every time step and if |IRMS| is two the RMS error will be calculated every other time step. If TOBS.INPUT is used, the RMS calculation will be performed for every constituent at the requested output grids (NGOUT), and if the TDDS is used, the error will be calculated for every constituent and grid requested with the TDDS input. The RMS errors are printed at the end of the output file. Model calibration will be discussed later.

The input variable IPLOT controls the options for storing the simulation results in direct access files. The first option is to store the grid concentrations at every time step in the direct access file GRID.DATA. Data from up to 199 time steps, including the initial conditions at time step zero, can be stored. The second storage option is to store parcel concentrations and locations in the direct access file PARCEL.DATA. At the conclusion of every time step the concentrations and location of every parcel are written. The formats of these storage files are given in Appendices D and E. The input variable IPLOT also controls whether a user-written subroutine PLOT will be called at the end of the simulation. PLOT is intended to be a plotting routine or a post-processor that uses data stored in the direct access files.

Tables of the decay coefficients S, XK, and CR can be included in the output. The number of specified coefficient outputs (NCO, maximum of twenty) is given for the simulation along with both a time and a grid output control value for each specified output. The output time control is accomplished with IPT. If IPT is greater than zero then output will occur at time step IPT, provided IPT is a multiple of IOUT, and if IPT is zero then output will occur at every normal output time step. Similarly, if the output grid control IPG is positive, and contained in NGOUT, output will occur for grid IPG and if IPG equals zero output will occur for all grids. Thus output can be specified for a particular time and grid, all times at one grid, one time at all grids, or all times at all grids.

APPLYING THE LAGRANGIAN TRANSPORT MODEL

This section discusses how to apply the LTM to practical problems. The model must be installed, all required input files must be prepared, the model run, and the output checked. Note that in order to run the LTM a decay-coefficient subroutine must be linked to the main program. Finally, the hydraulics, dispersion, and decay as defined by the model must be calibrated.

Availability of the Lagrangian Transport Model

The main LTM program, subroutines, documentation, installation instructions, and the example input and output files presented in this document are available from the U.S. Geological Survey Gulf Coast Hydrosience Center. The main program and the subroutines are listed in the LTM Programmers Manual (Schoellhamer and Jobson, 1986).

Input Files

At least one and possibly several input files may be needed by the LTM. These files are summarized in Table 2. The file LTM.INPUT sets up the simulation, defines the program options to be used, and defines the physical system being modeled. This file is always required. If the simulation is of unsteady flow the flow field must be read from either the file UNSTEADY.DATA or a TDDS time-dependent data base. The TDDS also requires a data station reference file that lists the station (grid point) identification numbers. If a root-mean-squared error is calculated the observed values must be read from either the file TOBS.INPUT or a TDDS time-dependent data base. If additional input is needed by the decay-coefficient subroutine then another input file may be needed. Examples of such a file are OXYGEN.INPUT in the oxygen modeling example of Appendix G and QUAL2.INPUT in Appendix H.

Output Files

The basic output is contained in file LTM.OUTPUT. This file presents some basic information about the simulation, the initial conditions in metric units, and the simulation results at the desired grid points and time interval. The results contain the time, grid number, travel time, grid concentrations, parcel concentration at entry, and change in concentration due to decay, dispersion, lateral inflows, and tributaries. If decay coefficient output has been requested, the tables will appear under the appropriate time and grid number, and if RMS calculations have been performed the results will be printed at the end of the file. As described previously, grid and parcel simulation results may be stored in direct

FILE ----	PURPOSE -----	APPENDIX -----
LTM.INPUT	Basic model input -- REQUIRED	A, ex: F, G, H
TOBS.INPUT	Observed concentrations for RMS	B, ex: F
UNSTEADY.DATA	Unsteady flow field	C, ex: G
decay.INPUT	Decay-coefficient subroutine input	ex: G, H
tddb	Time-dependent data base for TDDS	ex: G
DSRFILE	Data station reference file for TDDS	ex: G

Table 2.--Lagrangian Transport Model input files

access files and grid concentrations may also be stored in a time-dependent data base. The output files are summarized in Table 3.

Model Calibration

The first step in model calibration is to check the accuracy of the flow field. For steady flow simulations, the cross-sectional areas should be adjusted until the model travel times match the actual measured travel times. Considering that travel time equals the reach volume divided by the flow rate and that cross-sectional areas are read for grid points and converted to reach averaged values, adjust the cross-sectional areas at the two upstream grid points, A(1) and A(2), so that the travel time through reach one will be correct. Next adjust A(3) so that the travel time through reach two will be correct. Continue to proceed downstream adjusting areas to match reach travel times. Note that these areas are really effective flow areas and not actual cross-sectional areas. Ignoring travel times through small reaches can help eliminate oscillations in area that can propagate downstream. Since reach-averaged values are used in the model though, these oscillations do not affect the results.

For unsteady flow simulations the flow field is defined by velocities and areas at every grid point for every time step. One-dimensional unsteady flow models generally give results in terms of a mean velocity based on the discharge and cross-sectional area, so, if the flow model is calibrated correctly, the flow field given to the LTM will also be correct and no adjustment will be necessary. The BRANCH flow model (Schaffranek and others, 1981) was used by Schoellhamer and Curwick (1986) to generate flow fields for modeling sediment in the lower Mississippi River with the LTM. The BRANCH flow model is also used with the TDDS in the oxygen modeling example of Appendix G.

Once the correct areas or velocity/area combinations have been determined the top widths have to be calibrated if they are used in the decay-coefficient subroutine. In both the oxygen modeling and QUAL II reaction kinetics examples the cross-sectional area is divided by top width to get an average depth, so the top width should be adjusted to equate the average depth at each grid point to either a measured or calculated average depth.

The third step is to account for dispersion by calibrating the exchange flow ratio DQQ. The LTM reads DQQ for every reach in the system but often only one value is either known or calculated. If a longitudinal dispersion coefficient is known, equation 12 can be used to calculate a DQQ for steady flow and an approximate DQQ for unsteady flow. If a dye study has been performed or sufficient data on a conservative substance is available, the model can be used to find the DQQ that minimizes the RMS error. For the best results, DQQ should be between 0.1 and 0.4. The simulation time step should be adjusted to meet this recommendation because DQQ is a function of

FILE ----	PURPOSE -----	APPENDIX -----
LTM.OUTPUT	Basic model output	F, G, H
GRID.DATA	Grid concentrations at all time steps	D
PARCEL.DATA	Parcel concentrations and locations at all time steps	E
tddb	Time-dependent data base	G

Table 3.--Lagrangian Transport Model output files

both longitudinal dispersion and the time step. If possible, the simulation time step should also be selected such that parcel volumes are smaller than reach volumes between grid points.

The final step in the calibration process is to adjust the decay rates. If temperature is one of the constituents, calibrate it first and then calibrate the other constituents because their reaction coefficients are often functions of temperature. The simplified temperature algorithm developed by Jobson (1981) has been found to perform very well. This temperature algorithm is used in the oxygen modeling example and is included as comment lines in QUAL2.F77 of the QUAL II reaction kinetics example.

Several points about the calibration process are worth mentioning. First, the flow field must be well-calibrated for the model to accurately simulate the physical processes. Second, the calibration process is relatively simple due to the small number of non-decay coefficients (only DQQ's) that have to be adjusted. In addition, dispersion is often a minor factor in riverine water quality modeling so the solution may not be very sensitive to DQQ. Calibration of the decay coefficients, however, may be more involved depending on the complexity of the reaction kinetics and the desired model accuracy. Finally, a second set of independent data should be available to verify the calibrated model.

SUMMARY

A Users Manual for the Lagrangian Transport Model (LTM) has been presented. The LTM uses Lagrangian calculations that are based upon a reference frame moving with the river flow. The Lagrangian reference frame eliminates the need to numerically solve the convective term of the convection-diffusion equation and therefore provides significant numerical advantages over the more commonly used Eulerian reference frame. When properly applied, the LTM can simulate riverine transport and decay processes within the accuracy required by most water quality studies. The LTM is applicable to steady or unsteady one-dimensional unidirectional flows in fixed channels with tributary and lateral inflows. Application of the LTM is relatively simple and optional capabilities improve the model's convenience. Appendices give file formats and three example LTM applications that include the incorporation of the QUAL II water-quality model's reaction kinetics into the LTM.

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APPENDIX A

LTM.INPUT

File LTM.INPUT is the primary LTM input file and may be the only required input file. Each line of input is called a card and each card belongs to a data set. Each data set contains one type of information such as the title, cross-sectional areas, DQQ values, etc. A data set may contain one or more cards and the ordering of data sets must be as specified in this Appendix. Most data sets are always required and some data sets are to be included only in certain situations that are given with the data set. All cards have an identical format of ten spaces for card labeling (field zero) followed by ten seven-character fields of data except where noted otherwise. The card labels are written by the user to help the user identify the cards in the input files so the labels are not read by the program. All data can be justified anywhere within the field except for TDDS data types which must be right justified. The F7.0 input format for real numbers will correctly read any real number within the seven-character field and if a real number does not fit in a field the exponential (E) notation can be used to represent the number. Maximum values of some variables are given and all variables default to zero unless noted otherwise. Example LTM.INPUT files are presented in Appendices F, G, and H.

Data Set 1 -- Simulation Title

ALWAYS REQUIRED

Field	Variable	Format	Description
1	TITLE	80A1	Title of simulation

 Data Set 2 -- Simulation Control Card

ALWAYS REQUIRED

Field	Variable	Format	Description
0		10X	Card label
1	NXSEC	I7	Number of cross sections (grid points) in the simulation, MAXIMUM = 50
2	NIN(1)	I7	Number of tributary inflows (point sources) to be simulated
3	NIN(2)	I7	Number of lateral inflows (non point sources) to be simulated
4	Q	F7.0	Initial discharge at the upstream system boundary (Cu m or ft per sec)
5	HI	F7.0	Initial hour of the simulation in hours after midnight (for 7:30 PM, HI = 19.5)
6	NTS	I7	Number of time steps in the simulation, if grid data is to be stored the maximum NTS = 200
7	DT	F7.0	Simulation time step (Hours)
8	IUNSTD	I7	Defines steady/unsteady flow options: -steady state simulation, IUNSTD = 0 -unsteady simulation using UNSTEADY.DATA, IUNSTD = 1 -unsteady simulation using hydraulic and boundary condition data from the TDDS, IUNSTD = -1 -steady simulation using boundary conditions from the TDDS, IUNSTD = -2 -unsteady simulation using hydraulic data from the TDDS, IUNSTD = -3
9	NEQ	I7	Number of constituents in the simulation, MAXIMUM = 10
10	METRIC	I7	Defines the input data unit system: -English system (length=feet), METRIC=0 -Metric system (length=meters), METRIC=1

 Data Set 3 -- Output Control Card

ALWAYS REQUIRED

Field	Variable	Format	Description
0		10X	Card label
1	IOUT	I7	Time step interval at which output is desired
2	NGO	I7	Number of grids at which output is desired
3	IRMS	I7	Root mean squared error options: -No RMS calculation, IRMS = 0 -Time step interval at which error will be calculated = IRMS -Calculate RMS error using TOBS.INPUT, IRMS > 0 -Calculate RMS error using the TDDS, IRMS < 0
4	IPLOT	I7	Defines the store and PLOT option: -Do not store data, IPLOT = 0 -Store grid data, IPLOT = 1 -Store parcel data, IPLOT = 2 -Store both grid and parcel data, IPLOT = 3 -Do not call PLOT, IPLOT => 0 -Call user written subroutine PLOT, IPLOT < 0
5	NCO	I7	Number of decay coefficient outputs specified, MAXIMUM = 20
6-10			Empty

 Data Set 4 -- Output Grids

Include if $0 < \text{NGO} < \text{NXSEC}$, otherwise output at all grids

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	NGOUT(1)	I7	Grid number at which output is desired, in ascending order
2	NGOUT(2)	I7	Grid number at which output is desired, in ascending order
.	.	.	.
.	.	.	.
.	.	.	.
NGO	NGOUT(NGO)	I7	Grid number at which output is desired, in ascending order

 Data Set 5 -- Decay Coefficient Outputs

Include if NCO > 0

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	IPT(1)	I7	Time control for coefficient output 1: -Write output at regular time step interval IOUT, IPT(1) = 0 -Write output at time step IPT(1) (a multiple of IOUT), IPT(1) > 0
2	IPG(1)	I7	Grid control for coefficient output 1: -Write output at all regular output grids NGOUT, IPG(1) = 0 -Write output at grid IPG(1) (contained in array NGOUT), IPG(1) > 0
3, 5, 7,...	IPT(2...)	I7	Similar to field number one
4, 6, 8,...	IPG(2...)	I7	Similar to field number two
2*NCO-1	IPT(NCO)	I7	Similar to field number one
2*NCO	IPG(NCO)	I7	Similar to field number two

 Data Set 6 -- Constituent Label Card

ALWAYS REQUIRED

Field	Variable	Format	Description
0		10X	Card label
1	LABEL(1)	A7	Name of constituent number 1
2	LABEL(2)	A7	Name of constituent number 2
.	.	.	.
.	.	.	.
.	.	.	.
NEQ	LABEL(NEQ)	A7	Name of constituent number NEQ

 Data Set 7 -- River Miles or Kilometers of Grid Points

ALWAYS REQUIRED

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	X(1)	F7.0	River mi or km of grid point number 1, the upstream system boundary
2	X(2)	F7.0	River mi or km of grid point number 2, the grid point downstream from grid 1
.	.	.	.
.	.	.	.
.	.	.	.
NXSEC	X(NXSEC)	F7.0	River mi or km of grid point number NXSEC, the downstream system boundary

****NOTE:** River miles or kilometers are generally measured from the mouth of the river and must increase in the upstream direction. Thus $X(1) > X(2) > \dots > X(NXSEC)$.

 Data Set 8 -- Cross Sectional Areas

Include if simulation is of steady flow (IUNSTD = 0 or -2)

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	A(1)	F7.0	Cross sectional area at grid 1 (sq m or ft)
2	A(2)	F7.0	Cross sectional area at grid 2 (sq m or ft)
.	.	.	.
:	:	:	:
.	.	.	.
NXSEC	A(NXSEC)	F7.0	Cross sectional area at grid NXSEC (sq m or ft)

 Data Set 9 -- Top Widths

Include if simulation is of steady flow (IUNSTD = 0 or -2)

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	W(1)	F7.0	Top width at grid number 1 (m or ft)
2	W(2)	F7.0	Top width at grid number 2 (m or ft)
.	.	.	.
:	:	:	:
.	.	.	.
NXSEC	W(NXSEC)	F7.0	Top width at grid number NXSEC (m or ft)

****NOTE:** This data is only used by the decay coefficient subroutine. If top width is not used in the subroutine, (i.e. the conservative constituent example) then any values may be substituted and the card label(s) should note the substitution.

 Data Set 10 -- Tributary Inflows

Include if NIN(1) > 0

Field	Variable	Format	Description
-----	-----	-----	-----
0		10X	Card label, on all cards in data set
1	IGIN(1,1)	I7	Lowest grid number with a non-zero tributary inflow just downstream from the grid
2	FLOW(4,IGIN(1,1))	F7.0	Initial tributary discharge at grid IGIN(1,1) (cu m or ft per sec)
3, 5, 7,...	IGIN(2...,1)	I7	Grid number with non-zero tributary inflow just downstream from the grid, in ascending order
4, 6, 8,...	FLOW(4,IGIN(2...,1))	F7.0	Initial tributary discharge at corresponding grid (cu m or ft per sec)
2*NIN(1)-1	IGIN(NIN(1),1))	I7	Highest grid number with non-zero tributary inflow just downstream from the grid
2*NIN(1)	FLOW(4,IGIN(NIN(1),1))	F7.0	Initial tributary discharge at corresponding grid (cu m or ft per sec)

 Data Set 11 -- Lateral Inflows

Include if NIN(2) > 0

Field	Variable	Format	Description
-----	-----	-----	-----
0		10X	Card label, on all cards in data set
1	IGIN(1,2)	I7	Lowest grid number with a non-zero lateral inflow in the reach downstream from the grid
2	FLOW(5,IGIN(1,2))	F7.0	Initial lateral inflow downstream from grid IGIN(1,2) (sq m or ft per sec)
3, 5, 7,...	IGIN(2...,2)	I7	Grid number with non-zero lateral inflow in the reach downstream from the grid, in ascending order
4, 6, 8,...	FLOW(5,IGIN(2...,2))	F7.0	Initial lateral inflow downstream from the corresponding grid (sq m or ft per sec)
2*NIN(2)-1	IGIN(NIN(2),2)	I7	Highest grid number with non-zero lateral inflow in the reach downstream from the grid
2*NIN(2)	FLOW(5,IGIN(NIN(2),2))	F7.0	Initial lateral inflow at corresponding grid (sq m or ft per sec)

 Data Set 12 -- DQQ Values

ALWAYS REQUIRED

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	DQQ(1)	F7.0	DQQ value in the reach downstream from grid 1
2	DQQ(2)	F7.0	DQQ value in the reach downstream from grid 2
.	.	.	.
.	.	.	.
.	.	.	.
NXSEC	DQQ(NXSEC)	F7.0	DQQ value in the reach downstream from grid NXSEC

 Data Set 13 -- Initial Conditions

ALWAYS REQUIRED

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	GT(C,1)	F7.0	Initial concentration of constituent C at grid 1
2	GT(C,2)	F7.0	Initial concentration of constituent C at grid 2
.	.	.	.
.	.	.	.
.	.	.	.
NXSEC	GT(C,NXSEC)	F7.0	Initial concentration of constituent C at grid NXSEC

**Repeat Data Set 13 for each constituent (NEQ times), where C = 1 to NEQ.

 Data Set 14 -- TDDS Control Card

Include if TDDS is used

Field	Variable	Format	Description
0		10X	Card label
1	NINPUT	I7	Number of input data types for the simulation
2	NOUT	I7	Number of output data types for the simulation
3	LIST	I7	DADIO list option: -Print calender 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 15 -- TDDS Dates Card

Include if TDDS is used

Field	Variable	Format	Description
0		10X	Card label
1	BY	I7	Beginning year of simulation (i.e. '85')
2	BMO	I7	Beginning month of simulation
3	BD	I7	Beginning day of simulation
4	BH	I7	Beginning hour of simulation (0,...,23)
5	BMN	I7	Beginning minute of simulation
6	EY	I7	Ending year of simulation (i.e. '85')
7	EMO	I7	Ending month of simulation
8	ED	I7	Ending day of simulation
9	EH	I7	Ending hour of simulation (0,...,23)
10	EMN	I7	Ending minute of simulation

 Data Set 16 -- TDDS Station Identification

Include if TDDS is used

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

 Data Set 17 -- TDDS Input

Include if NINPUT > 0

Field	Variable	Format	Description
-----	-----	-----	-----
0		10X	Card label, on all cards in data set
1	INTYPE(I)	5X,A2	TDDS data type (see Table 2-1)
2	RDPDY(I)	I7	Readings per day of INTYPE(I) in TDDS, DEFAULT = simulation time steps per day
3	NINGRD(I)	I7	Number of grids with INTYPE(I), DEFAULT = NXSEC
4	INGRID(1,I)	I7	Lowest grid number with INTYPE(I), omit only if NINGRD(I) is omitted (defaults to 1)
5	INGRID(2,I)	I7	Grid number with INTYPE(I) in ascending order, omit only if NINGRD(I) is omitted (defaults to 2)
.	.	.	.
.	.	.	.
.	.	.	.
3+NINGRD(I)	INGRID(NINGRD(I),I)	I7	Highest grid number with INTYPE(I), omit only if NINGRD(I) is omitted (defaults to NXSEC)

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

 Data Set 18 -- TDDS Output

Include if NOUT > 0

Field	Variable	Format	Description
-----	-----	-----	-----
0		10X	Card label, on all cards in data set
1	OUTTYP(J)	5X,A2	Output data type, see Table 5-1
2	NOUTGR(J)	I7	Number of grids with OUTTYP(J), DEFAULT = NXSEC-1
3	OUTGRD(1,J)	I7	Lowest grid number with OUTTYP(J), omit only if NOUTGR(J) is omitted (defaults to 2)
4	OUTGRD(2,J)	I7	Grid number with OUTTYP(J) in ascending order, omit only if NOUTGR(J) is omitted (defaults to 3)
.	.	.	.
:	:	:	:
.	.	.	.
2+OUTGRD(J)	OUTGRD(NOUTGR(J),J)	I7	Highest grid number with OUTTYP(J), omit only if NOUTGR(J) is omitted (defaults to NXSEC)

**Repeat data set NOUT times where J = 1 to NOUT.

 Data Set 19 -- Boundary Conditions

Include if boundary conditions are not read with the TDDS

Field	Variable	Format	Description
-----	-----	-----	-----
0		10X	Card label, on all cards in data set
1	TUP(C)	F7.0	Concentration of constituent C at the upstream boundary
2	CIN(C,IGIN(1,1),1)	F7.0	Concentration of constituent C in tributary inflow at grid IGIN(1,1)
3	CIN(C,IGIN(2,1),1)	F7.0	Concentration of constituent C in tributary inflow at grid IGIN(2,1)
:	:	:	:
:	:	:	:
:	:	:	:
1+NIN(1)	CIN(C,IGIN(NIN(1),1),1)	F7.0	Concentration of constituent C in tributary inflow at grid IGIN(NIN(1),1)
2+NIN(1)	CIN(C,IGIN(1,2),2)	F7.0	Concentration of constituent C in lateral inflow in the reach downstream from grid IGIN(1,2)

(continued on the next page)

Field -----	Variable -----	Format -----	Description -----
3+NIN(1)	CIN(C,IGIN(2,2),2)	F7.0	Concentration of constituent C in lateral inflow in the reach downstream from grid IGIN(2,2)
.	.	.	.
.	.	.	.
.	.	.	.
1+NIN(2)+NIN(1)	CIN(C,IGIN(NIN(2),2),2)	F7.0	Concentration of constituent C in lateral inflow in the reach downstream from grid IGIN(NIN(2),2)

**Repeat for every constituent (NEQ times) where C = 1 to NEQ.

**Repeat data set for every time step (NTS times).

**Average values during the time step must be provided.

APPENDIX B

TOBS.INPUT

File TOBS.INPUT is used to provide observed concentrations to the LTM for the calculation of a root mean squared error when IRMS = 1. No RMS calculation will be made with a negative concentration read from this file. Every card has a format of ten spaces for card labeling followed by ten F7.0 fields. The file format is given in this Appendix. An example TOBS.INPUT is listed in Appendix F.

Field	Variable	Format	Description
0		10X	Card label, on all cards in file
1	TACT(C,1)	F7.0	Actual concentration of constituent C at grid NGOUT(1) and time step IRMS
2	TACT(C,2)	F7.0	Actual concentration of constituent C at grid NGOUT(2) and time step IRMS
.	.	.	.
.	.	.	.
.	.	.	.
NGO	TACT(C,NGO)	F7.0	Actual concentration of constituent C at grid NGOUT(NGO) and time step IRMS

**Repeat for each constituent C where C = 1 to NEQ for time step IRMS with TACT(C,1) always in field 1.

**Repeat for all NGOUT and constituents at time steps 2*IRMS, 3*IRMS...

APPENDIX C

UNSTEADY.DATA

If unsteady flow is to be simulated, then the flow field must be provided from either the TDDS or the file UNSTEADY.DATA which contains the flow field for every grid and every time step. Unlike the other input files discussed, UNSTEADY.DATA has a format of ten eight character fields per line. The flow field data stored in the file are velocity (m/sec or ft/sec), area (m² or ft²), top width (m or ft), tributary inflow just below the corresponding grid (m³/sec or ft³/sec), and lateral inflow in the reach below the grid point (m²/sec or ft²/sec). As mentioned in Appendix A, top width may or may not be used for calculations, depending on the decay coefficient subroutine. Any value may be used for top width if it is not used, although this may be misleading at a later date.

Field	Variable	Format	Description
-----	-----	-----	-----
5*(G-1)+1	FLOW(1,G)	F8.0	Velocity at grid G (m or ft/hr), G = 1 to NXSEC
5*(G-1)+2	FLOW(2,G)	F8.0	Cross sectional area at grid G (sq m or ft), G = 1 to NXSEC
5*(G-1)+3	FLOW(3,G)	F8.0	Top width at grid G (m or ft), G = 1 to NXSEC
5*(G-1)+4	FLOW(4,G)	F8.0	Tributary inflow just downstream from grid G (cu m or ft per sec), G = 1 to NXSEC
5*(G-1)+5	FLOW(5,G)	F8.0	Lateral inflow in the reach downstream from grid G (sq m or ft per sec), G = 1 to NXSEC

**Repeat NTS+1 times, beginning with the initial conditions and proceeding up to time step NTS. FLOW(1,1) is always in field number 1. Data for two grids is on each line.

APPENDIX D

GRID.DATA

File GRID.DATA is a direct access file created when requested with the variable IPLOT. The file contains grid concentrations for every grid and every time step and has a record length of 400 words. The primary purpose of GRID.DATA is to provide data to the user-written subroutine PLOT, but it can also be used to store data for subsequent plotting or for future reference. The initial conditions and up to 199 additional time steps of data may be stored. The file format is given in this Appendix.

Record	Description
-----	-----
1	Concentrations of constituent 1 at grid 1, beginning from simulation time zero (initial condition) and proceeding up to time step NTS, where $NTS < 200$
2	Concentrations of constituent 2 at grid 1, beginning from simulation time zero (initial condition) and proceeding up to time step NTS, where $NTS < 200$
.	.
.	.
.	.
NEQ	Concentrations of constituent NEQ at grid 1, beginning from simulation time zero (initial condition) and proceeding up to time step NTS, where $NTS < 200$
NEQ+1	Concentrations of constituent 1 at grid 2, beginning from simulation time zero (initial condition) and proceeding up to time step NTS, where $NTS < 200$
.	.
.	.
.	.
NEQ*(G-1)+C	Concentrations of constituent C at grid G, beginning from simulation time zero (initial condition) and proceeding up to time step NTS, where $NTS < 200$
.	.
.	.
.	.
NEQ*NXSEC	Concentrations of constituent NEQ at grid NXSEC, beginning from simulation time zero (initial condition) and proceeding up to time step NTS, where $NTS < 200$

APPENDIX E

PARCEL.DATA

File PARCEL.DATA is a direct access file (record length of 1000 words) created when requested with the input variable IPLOT. The file contains parcel concentrations and locations for every parcel at the end of every time step. The primary purpose of PARCEL.DATA is to provide data to the user-written subroutine PLOT, but it can also be used to store data for plotting after the LTM run or for future reference. Unlike GRID.DATA, there is no limit to the number of time steps that can be stored, so this file can be very large. The file format is given in this Appendix.

Record	Description
1	Parcel concentrations of constituent 1 at time step zero (initial condition), proceeding from the most upstream parcel (1) to the most downstream parcel
2	Parcel concentrations of constituent 2 at time step zero (initial condition), proceeding from the most upstream parcel (1) to the most downstream parcel
.	.
.	.
.	.
NEQ	Parcel concentrations of constituent NEQ at time step zero (initial condition), proceeding from the most upstream parcel (1) to the most downstream parcel
NEQ+1	Parcel locations (upstream locations) at time step zero (initial condition) in grid coordinates, proceeding from the most upstream parcel (1) to the most downstream parcel
.	.
.	.
.	.
T*(NEQ+1)+C	Parcel concentrations of constituent C at time step T, proceeding from the most upstream parcel (1) to the most downstream parcel
(T+1)*(NEQ+1)	Parcel locations (upstream locations) at time step T, proceeding from the most upstream parcel (1) to the most downstream parcel
.	.
.	.
.	.
NTS*(NEQ+1) +NEQ	Parcel concentrations of constituent NEQ at time step NTS, proceeding from the most upstream parcel (1) to the most downstream parcel
(NTS+1)* (NEQ+1)	Parcel locations (upstream locations) at the end of time step NTS, proceeding from the most upstream parcel (1) to the most downstream parcel

APPENDIX F

CONSERVATIVE CONSTITUENT EXAMPLE

A conservative constituent does not decay with time. Salinity and metals are often assumed to be conservative water-quality constituents. Dye used in travel-time studies is theoretically conservative and is simulated in this example.

Yotsukura and others (1970) used dye to measure longitudinal dispersion in the reach of the Missouri River between Sioux City, Iowa (river mile 732) and Plattsmouth, Nebraska (river mile 591) shown in Figure 5. The steady discharge was approximately 33,300 ft³/s and no appreciable inflows or outflows were present in the study area. Dye was injected as a slug at Combination Bridge in Sioux City and the passage of the resulting dye cloud was measured at four downstream cross sections. The authors concluded that, for this reach of river and flow condition, the longitudinal dispersion coefficient obtained between Blair and Plattsmouth (16,000 ft²/s) is the best approximation obtainable by the routing method. A value of 15,000 ft²/s was obtained by the method of moments for the entire reach.

This data is used to verify the LTM by matching the model results to the measured results and back calculating dispersion coefficients with equation 12. The LTM dispersion coefficient should approximate the previous results. This Appendix describes how the LTM was applied and presents the input and output files from the model run that produced the best fit of the actual data.

The LTM was prepared by loading the main program LTM.F77 with the conservative decay-coefficient subroutine CON.F77 which is listed in the LTM Programmers Manual (Schoellhamer and Jobson, 1986). CON.F77 can simulate up to ten conservative constituents and this file also contains instructions for converting it to independently decay up to ten constituents with first order reactions. This Appendix contains the input files LTM.INPUT and TOBS.INPUT and the output file CONSERVATIVE.OUTPUT of the calibrated model. The values in file CONSERVATIVE.OUTPUT will be discussed in detail later in this Appendix. Unlike the other two decay-coefficient subroutines presented in this document, CON.F77 does not require a separate input file unless the first order independent decay option is used.

The LTM poorly models injection of a slug of dye because the slug must initially be diluted in a parcel which artificially increases the model's dispersion. So the upstream boundary of the LTM simulation was taken at the most upstream point at which the dye cloud was measured (Decatur Highway Bridge at river mile 691). These dye concentrations were used as the upstream boundary condition for the LTM. Five other grid points were included in the simulation, three at which dye concentrations and hydraulic

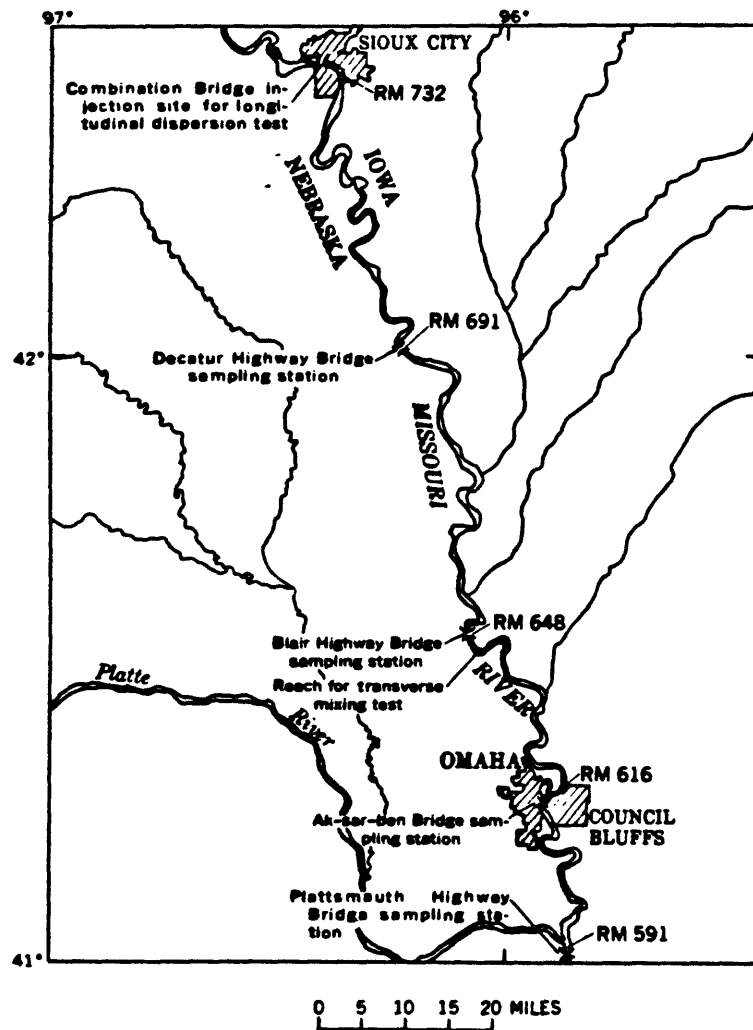


Figure 5.--Missouri River study reach, between Sioux City, Iowa, and Plattsmouth, Nebraska, (from Yotsukura and others, 1970)

data were recorded and two at which only hydraulic data were recorded. All measured dye concentrations on the tail of a dye cloud and below three percent of the peak concentration were truncated (Yotsukura and others, 1970). The dye concentrations used for the upstream boundary conditions were the average concentrations during each time step while the observed concentrations, corrected for dye loss, used for the RMS calculations were at the end of the time step. The simulation time step was 0.5 hours, which produced a DQQ value for the entire system in the desired 0.1 to 0.4 range.

The three downstream grid points at which dye concentrations were measured were used to calibrate the LTM. First, cross-sectional areas were adjusted slightly so that the peak LTM concentrations at the three grid points occurred at the same time as the measured peak concentrations. Once the hydraulics were closely matched, DQQ was adjusted until the root-mean-squared error of the LTM results was minimized at the three grid points with measured concentrations. The optimal value of DQQ is 0.25.

The optimum LTM.INPUT file is listed in this Appendix and the format is given in Appendix A. Following the title card is the simulation control card. Proceeding from left to right on this card, the system is composed of 6 grid points, no tributaries or lateral inflows, and an upstream discharge of 33,300 ft³/s. The simulation starts 10.5 hours after midnight and has 79 time steps of 0.5 hours each. The simulation is of steady flow (IUNSTD = 0) with 1 constituent and the input data are in English units (METRIC = 0). The output control card specifies that output be printed every 2 time steps, that output is desired at 3 grid points, the RMS error is to be calculated every time step with data from TOBS.INPUT (IRMS = 1), and no data storage (IPLLOT = 0) and no decay-coefficient output (NCO = 0) are desired. Output is desired at grids 3, 5, and 6, at which dye concentrations were measured. The modeled constituent is dye. The river miles, cross-sectional areas, top widths, exchange flow ratio DQQ, and initial conditions follow. As previously mentioned, even though a top widths data set is required because the flow is steady, the given values are not used in this simulation because they are not used in the decay coefficient subroutine. The remainder of LTM.INPUT contains the dye concentration at the upstream boundary of the system for each time step.

Figure 6 shows the measured and optimum simulated concentration profiles. A discrepancy occurs because the recovery ratio of dye at Plattsmouth Bridge was lower than at the other cross sections. This could have been corrected in the decay-coefficient subroutine by allowing dye to decay in the reach above Plattsmouth Bridge.

In order to calculate longitudinal dispersion coefficients from the model results, representative velocities must be determined for use in equation 12. These velocities were determined by dividing the distance between the upstream and downstream boundaries of the reach in question by the travel time between those two points. Between Blair and Plattsmouth a mean velocity of 5.77 ft/sec and a longitudinal dispersion coefficient of

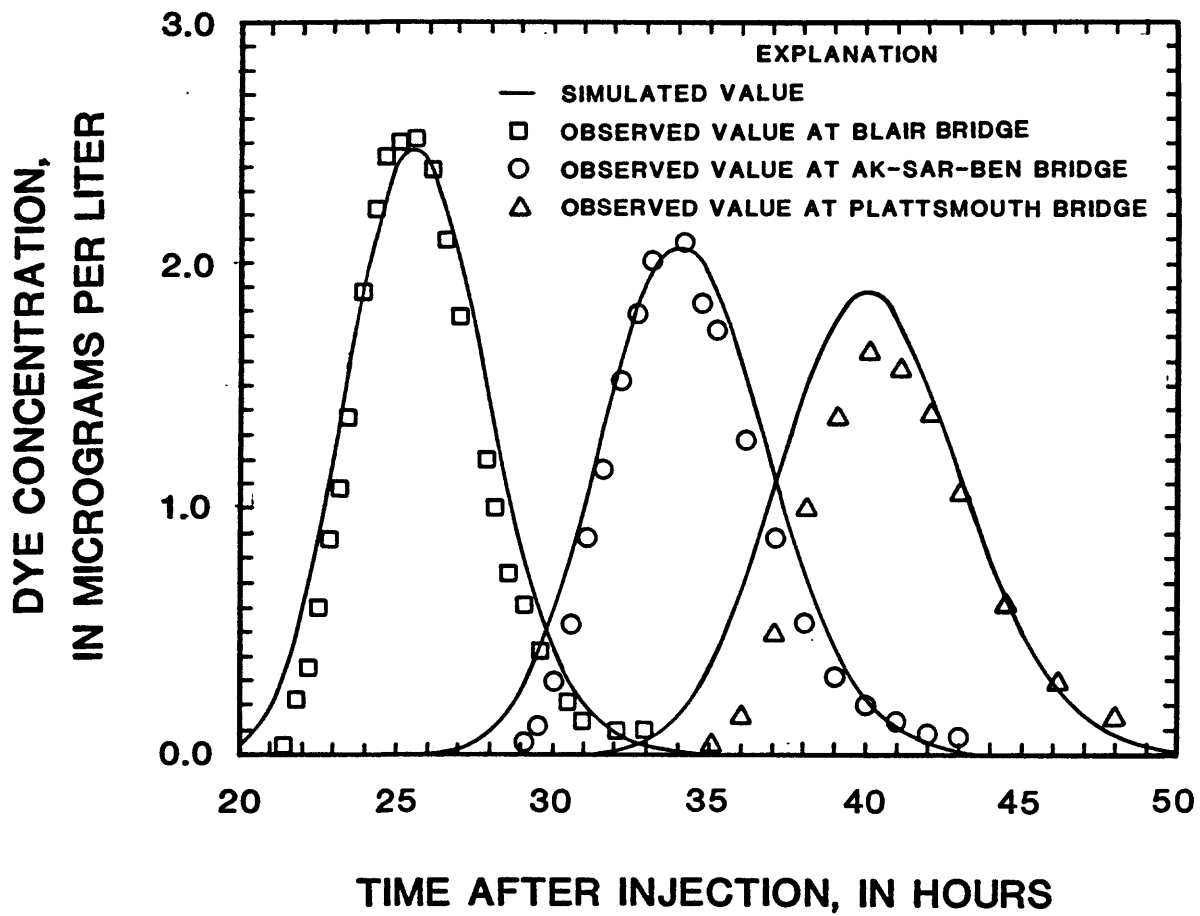


Figure 6.--Missouri River dye concentration profiles

approximately 15,000 ft²/s resulted. Between Decatur and Plattsmouth a mean velocity of 5.49 ft/sec and a longitudinal dispersion coefficient of approximately 13,500 ft²/s resulted. These synthetic dispersion coefficients compare favorably with the measured values of 16,000 and 15,000 ft²/s, respectively.

52

BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0
BC	0.0

OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.000	0.000	0.000
OBSDYE@356	0.010	0.000	0.000
OBSDYE@356	0.020	0.000	0.000
OBSDYE@356	0.290	0.000	0.000
OBSDYE@356	0.600	0.000	0.000
OBSDYE@356	1.090	0.000	0.000
OBSDYE@356	1.580	0.000	0.000
OBSDYE@356	2.050	0.000	0.000
OBSDYE@356	2.450	0.000	0.000
OBSDYE@356	2.500	0.000	0.000
OBSDYE@356	2.520	0.000	0.000
OBSDYE@356	2.390	0.000	0.000
OBSDYE@356	2.050	0.000	0.000
OBSDYE@356	1.780	0.000	0.000
OBSDYE@356	1.300	0.000	0.000
OBSDYE@356	1.010	0.000	0.000
OBSDYE@356	0.740	0.000	0.000
OBSDYE@356	0.610	0.040	0.000
OBSDYE@356	0.420	0.110	0.000
OBSDYE@356	0.300	0.290	0.000
OBSDYE@356	0.210	0.530	0.000
OBSDYE@356	0.140	0.880	0.000
OBSDYE@356	0.120	1.160	0.000
OBSDYE@356	0.090	1.520	0.000
OBSDYE@356	0.090	1.790	0.000
OBSDYE@356	0.090	2.010	0.000
OBSDYE@356	0.000	2.050	0.000
OBSDYE@356	0.000	2.090	0.000
OBSDYE@356	0.000	1.840	0.010
OBSDYE@356	0.000	1.730	0.030
OBSDYE@356	0.000	1.530	0.090
OBSDYE@356	0.000	1.280	0.150
OBSDYE@356	0.000	1.080	0.320
OBSDYE@356	0.000	0.880	0.490
OBSDYE@356	0.000	0.710	0.750
OBSDYE@356	0.000	0.540	1.000
OBSDYE@356	0.000	0.430	1.190
OBSDYE@356	0.000	0.320	1.370
OBSDYE@356	0.000	0.260	1.500
OBSDYE@356	0.000	0.200	1.640
OBSDYE@356	0.000	0.170	1.610
OBSDYE@356	0.000	0.130	1.570
OBSDYE@356	0.000	0.110	1.480
OBSDYE@356	0.000	0.090	1.390
OBSDYE@356	0.000	0.080	1.230
OBSDYE@356	0.000	0.070	1.070
OBSDYE@356	0.000	0.060	0.920
OBSDYE@356	0.000	0.000	0.770
OBSDYE@356	0.000	0.000	0.620
OBSDYE@356	0.000	0.000	0.520
OBSDYE@356	0.000	0.000	0.420
OBSDYE@356	0.000	0.000	0.320
OBSDYE@356	0.000	0.000	0.250
OBSDYE@356	0.000	0.000	0.220
OBSDYE@356	0.000	0.000	0.200
OBSDYE@356	0.000	0.000	0.150
OBSDYE@356	0.000	0.000	0.130

Appendix F**Conservative Constituent****TOBS.INPUT**

OBSDYE@356	0.000	0.000	0.110
OBSDYE@356	0.000	0.000	0.090
OBSDYE@356	0.000	0.000	0.080

MISSOURI RIVER TEST -- MSP 1899-G

SIMULATION IS OF STEADY FLOW

INPUT DATA IS ENGLISH

MODEL IS TO RUN 79 TIME STEPS EACH 0.50 HOURS LONG.

THE SIMULATION STARTS 10.5000 HOURS AFTER MIDNIGHT.

THE RIVER IS DISCRETIZED BY 6 GRID POINTS.

THE INITIAL UPSTREAM DISCHARGE IS CONSTANT AT 33300.00 CUBIC METERS OR FEET PER SEC.

EVERY 2 TIME STEPS DATA WILL BE PRINTED FOR THE FOLLOWING GRIDS:

3 5 6

THE CONSTITUENTS MODELED ARE:

1 DYE

INITIAL CONDITIONS

GRID	RIVER KM	TRIB. FLOW CU M/SEC	VELOCITY M/HR	AREA SQ M	TOP WIDTH METERS	LAT FLOW SQ M/S	DISP FACT DQQ	INITIAL CONCENTRATIONS OF CONSTITUENTS 1
1	1112.05	0.000						0.0
2	1078.26	0.000	5430.6	625.09	184.40	0.000000	0.25	0.0
3	1042.85	0.000	5893.2	576.02	182.88	0.000000	0.25	0.0
4	1038.02	0.000	6155.0	551.52	204.22	0.000000	0.25	0.0
5	991.35	0.000	5986.8	567.02	200.71	0.000000	0.25	0.0
6	951.12	0.000	6807.1	498.69	177.09	0.000000	0.25	0.0

Appendix F

Conservative Constituent CONSERVATIVE.OUTPUT

TIME DAY	HOUR	GRID NUMBER	TRAVEL TIME(HR)	CONSTITUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			
							DECAY	DISP	LATQ	TRIB
1	11.50	3	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	12.50	3	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	13.50	3	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	14.50	3	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	15.50	3	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	16.50	3	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	17.50	3	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	18.50	3	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00

Appendix F

Conservative Constituent CONSERVATIVE.OUTPUT

TIME DAY	HOUR	GRID NUMBER	TRAVEL TIME(HR)	CONSTITUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			
							DECAY	DISP	LATQ	TRIB
1	19.50	3	0.00	DYE	0.01	0.00	0.00	0.01	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	20.50	3	0.00	DYE	0.08	0.00	0.00	0.08	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	21.50	3	0.00	DYE	0.34	0.00	0.00	0.34	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	22.50	3	0.00	DYE	0.91	0.00	0.00	0.91	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
1	23.50	3	12.23	DYE	1.68	1.45	0.00	0.23	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
2	0.50	3	12.23	DYE	2.29	3.52	0.00	-1.23	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
2	1.50	3	12.23	DYE	2.48	3.84	0.00	-1.36	0.00	0.00
		5	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
2	2.50	3	12.23	DYE	2.19	2.74	0.00	-0.55	0.00	0.00
		5	0.00	DYE	0.01	0.00	0.00	0.01	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00

Appendix F

Conservative Constituent CONSERVATIVE.OUTPUT

TIME DAY	TIME HOUR	GRID NUMBER	TRAVEL TIME(HR)	CONSTITUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			
							DECAY	DISP	LATQ	TRIB
2	3.50	3	12.23	DYE	1.64	1.38	0.00	0.26	0.00	0.00
		5	0.00	DYE	0.04	0.00	0.00	0.04	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
2	4.50	3	12.23	DYE	1.05	0.59	0.00	0.46	0.00	0.00
		5	0.00	DYE	0.14	0.00	0.00	0.14	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
2	5.50	3	12.23	DYE	0.60	0.23	0.00	0.37	0.00	0.00
		5	0.00	DYE	0.39	0.00	0.00	0.39	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
2	6.50	3	12.23	DYE	0.30	0.00	0.00	0.30	0.00	0.00
		5	0.00	DYE	0.81	0.00	0.00	0.81	0.00	0.00
		6	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
2	7.50	3	12.23	DYE	0.13	0.00	0.00	0.13	0.00	0.00
		5	20.81	DYE	1.33	0.40	0.00	0.93	0.00	0.00
		6	0.00	DYE	0.01	0.00	0.00	0.01	0.00	0.00
2	8.50	3	12.23	DYE	0.05	0.00	0.00	0.05	0.00	0.00
		5	20.81	DYE	1.80	2.66	0.00	-0.86	0.00	0.00
		6	0.00	DYE	0.03	0.00	0.00	0.03	0.00	0.00
2	9.50	3	12.23	DYE	0.02	0.00	0.00	0.02	0.00	0.00
		5	20.81	DYE	2.05	3.98	0.00	-1.93	0.00	0.00
		6	0.00	DYE	0.09	0.00	0.00	0.09	0.00	0.00
2	10.50	3	12.23	DYE	0.01	0.00	0.00	0.01	0.00	0.00
		5	20.81	DYE	2.02	3.37	0.00	-1.35	0.00	0.00
		6	0.00	DYE	0.23	0.00	0.00	0.23	0.00	0.00

Appendix F

Conservative Constituent CONSERVATIVE.OUTPUT

TIME		GRID NUMBER	TRAVEL TIME(HR)	CONSTITUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			
DAY	HOOR						DECAY	DISP	LATQ	TRIB
2	11.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	20.81	DYE	1.74	2.01	0.00	-0.27	0.00	0.00
		6	0.00	DYE	0.50	0.00	0.00	0.50	0.00	0.00
2	12.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	20.81	DYE	1.33	0.92	0.00	0.41	0.00	0.00
		6	0.00	DYE	0.88	0.00	0.00	0.88	0.00	0.00
2	13.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	20.81	DYE	0.91	0.36	0.00	0.55	0.00	0.00
		6	26.72	DYE	1.31	0.40	0.00	0.91	0.00	0.00
2	14.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	20.81	DYE	0.56	0.14	0.00	0.42	0.00	0.00
		6	26.72	DYE	1.67	2.66	0.00	-0.99	0.00	0.00
2	15.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	20.81	DYE	0.32	0.00	0.00	0.32	0.00	0.00
		6	26.72	DYE	1.86	3.98	0.00	-2.12	0.00	0.00
2	16.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	20.81	DYE	0.16	0.00	0.00	0.16	0.00	0.00
		6	26.72	DYE	1.84	3.37	0.00	-1.53	0.00	0.00
2	17.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	20.81	DYE	0.08	0.00	0.00	0.08	0.00	0.00
		6	26.72	DYE	1.62	2.01	0.00	-0.39	0.00	0.00
2	18.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
		5	20.81	DYE	0.03	0.00	0.00	0.03	0.00	0.00
		6	26.72	DYE	1.30	0.92	0.00	0.38	0.00	0.00

Appendix F

Conservative Constituent CONSERVATIVE.OUTPUT

TIME DAY HOUR	GRID NUMBER	TRAVEL TIME(HR)	CONSTITUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			
						DECAY	DISP	LATQ	TRIB
2 19.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	5	20.81	DYE	0.01	0.00	0.00	0.01	0.00	0.00
	6	26.72	DYE	0.94	0.36	0.00	0.58	0.00	0.00
2 20.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	5	20.81	DYE	0.01	0.00	0.00	0.01	0.00	0.00
	6	26.72	DYE	0.62	0.14	0.00	0.48	0.00	0.00
2 21.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	5	20.81	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	6	26.72	DYE	0.38	0.00	0.00	0.38	0.00	0.00
2 22.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	5	20.81	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	6	26.72	DYE	0.22	0.00	0.00	0.22	0.00	0.00
2 23.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	5	20.81	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	6	26.72	DYE	0.11	0.00	0.00	0.11	0.00	0.00
3 0.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	5	20.81	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	6	26.72	DYE	0.06	0.00	0.00	0.06	0.00	0.00
3 1.50	3	12.23	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	5	20.81	DYE	0.00	0.00	0.00	0.00	0.00	0.00
	6	26.72	DYE	0.03	0.00	0.00	0.03	0.00	0.00

CONSTITUENT RMS ERROR
DYE 0.13429

APPENDIX G

OXYGEN MODELING EXAMPLE

This Appendix presents an application of the LTM using unsteady flow data from the TDDS. This flow data was generated by applying the BRANCH flow model (Schaffranek and others, 1981) to the 13.8 mile reach of the Ohio River along the Kentucky and Ohio border below Greenup Dam shown in Figure 7. The water-quality data is hypothetical. Four constituents are simulated -- conservative dye, temperature, biochemical oxygen demand (BOD), and dissolved oxygen (DO). Dye is used to 'calibrate' model dispersion with 'measured' dye data, similar to the procedure in Appendix F. Temperature is modeled to help determine the rate coefficients for the oxygen reactions.

The files LTM.INPUT, OXYGEN.INPUT and OXYGEN.OUTPUT are listed in this Appendix. The decay-coefficient subroutine OXYGEN.F77 is listed in the LTM Programmers Manual (Schoellhamer and Jobson, 1986) and the subroutine's reaction kinetics will be described in this Appendix. The file OXYGEN.INPUT is the input file for OXYGEN.F77.

Temperature is modeled with Jobson's simplified temperature algorithm (1981). Temperature decays according to

$$\frac{\partial T}{\partial t} = \frac{-B}{A \rho c_p} K(T - T_a) \quad (15)$$

where K is a function of water temperature and wind speed, T is the water temperature (Celsius), T_a is either the equilibrium water temperature or the air temperature (Celsius), B is the cross-sectional top width, ρ is the density of water, and c_p is the specific heat of water.

BOD is assumed to decay as a first order reaction. Thus

$$\frac{\partial BOD}{\partial t} = -K_1 * BOD \quad (16)$$

in which K_1 is the first order BOD decay coefficient.

The source of dissolved oxygen in the model is reaeration that is modeled as a first order reaction. The dissolved oxygen sinks are BOD consumption which is equal to the BOD decay rate and benthic demand that is assumed to be constant. Thus dissolved oxygen decays according to

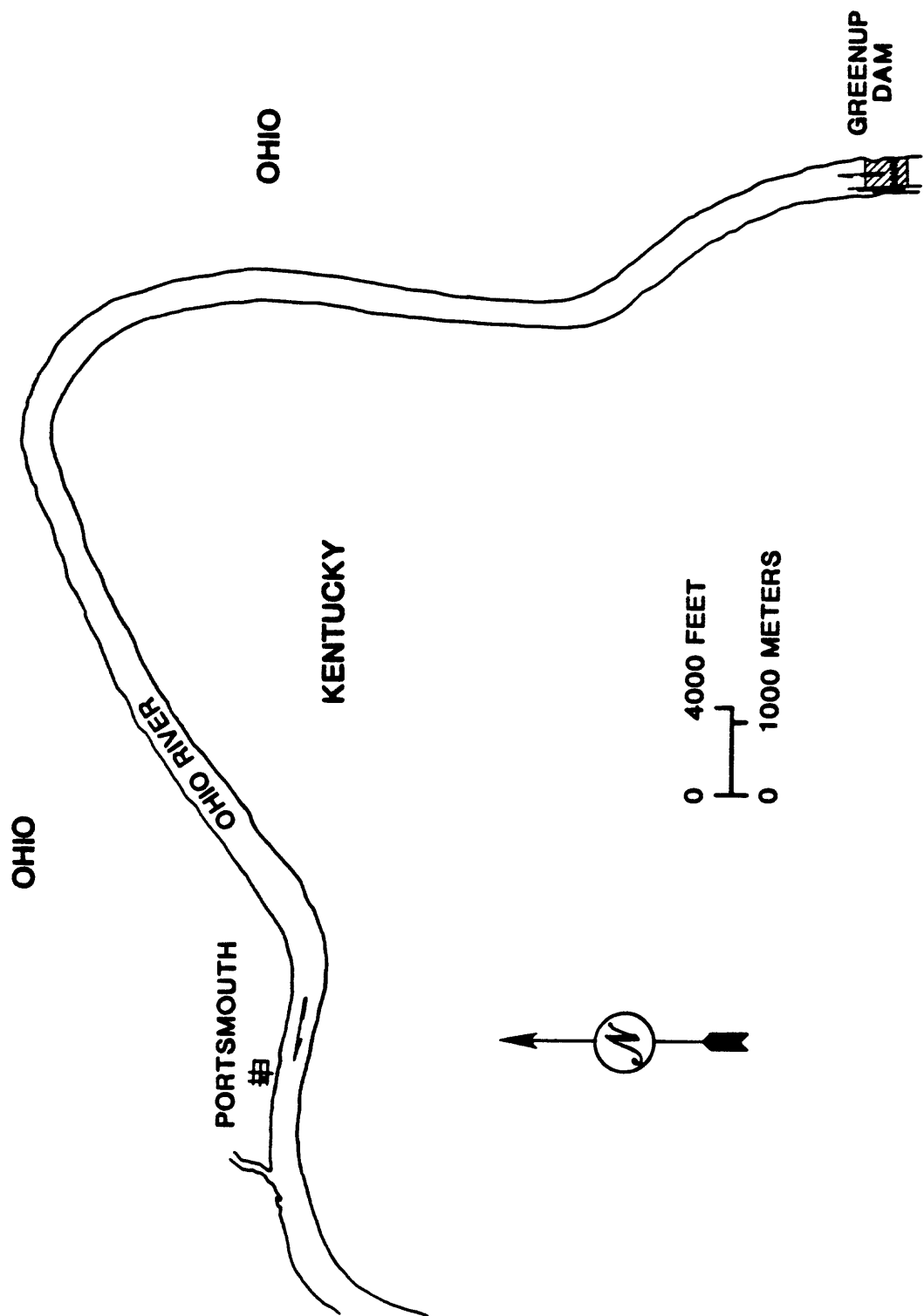


Figure 7.--Ohio River study reach, between Greenup Dam and Portsmouth, Ohio.

$$\frac{\partial DO}{\partial t} = -K_1 * BOD - \frac{K_4}{A} + K_2 * (DO - CR_{DO}) \quad (17)$$

where K_2 is the temperature dependent reaeration coefficient (1/day), K_4 is the benthos source rate for BOD (mg/day/ft), and CR_{DO} is the equilibrium or saturation concentration of dissolved oxygen (mg/L) that is determined with the empirical relationship

$$CR_{DO} = \frac{468.0}{T + 31.6} \quad (18)$$

Both K_1 and K_2 are temperature dependent. This dependency is represented by

$$K_T = K_{20} (T - 20)^\theta \quad (19)$$

in which K_T is the temperature corrected coefficient, K_{20} is the value of the temperature dependent coefficient at 20°C, and θ is a constant equal to 1.047 for K_1 and 1.0159 for K_2 .

The LTM is prepared by loading the main program LTM.F77, the decay-coefficient subroutine OXYGEN.F77, and the Time-Dependent Data System interface subroutine TDDS.F77.

The LTM.INPUT file is listed in this Appendix and the format is given in Appendix A. After the title card the simulation control card specifies a system with 8 grid points, no tributary or lateral inflows, and an initial upstream discharge of 77,850 ft³/s. The simulation starts 6.0 hours after midnight and has 48 time steps of 0.25 hours each. The simulation is of unsteady flow read from the TDDS (IUNSTD = -1) with 4 constituents and the input data is in English units (METRIC = 0). The next two cards specify that output will be printed every 24 time steps, output is desired at every grid point (NGO = NXSEC = 8), the RMS error is to be calculated with data from the TDDS every time step (IRMS = -1), no data is to be stored (IPLOT = 0), and one decay-coefficient output is desired (NCO = 1) during time step 24 at grid 6. Next the constituent names, river miles, DQQ (0.34 was the 'optimum' DQQ), and initial conditions are given. The TDDS control card specifies that 10 TDDS input data types are to be read, no TDDS data types are to be written to the TDDS, and the TDDS index directory is to be printed (LIST = 1). The beginning and ending times of the simulation and the TDDS station numbers are given. Finally, each TDDS input data type is listed. Data types Q (discharge), A (cross-sectional area), and B (cross-sectional top width) are stored in the TDDS with 48 readings per day and input is requested at all eight grid points because the default values are used. Data types C1 (dye concentration) and M1 (measured dye concentration) are stored with 96 readings per day and C1 is desired at grid number 1 (the

upstream boundary) only while M1 is desired at grid 8 (the downstream boundary) at which the RMS error calculation will be performed. Data types C2, C3, and C4 contain the upstream boundary conditions for temperature, BOD, and dissolved oxygen, respectively. Data types AT and WS are the air temperature and wind speed that are read at grid one but applied throughout the system.

Figure 8 shows discharge plotted against time at the upstream boundary. Constant dye injection at the upstream boundary produced dye concentrations of 10.00, 9.84, 9.67, and 9.51 mg/L during the time steps that begin at 6:00 AM, 6:15 AM, 6:30 AM, and 6:45 AM, respectively. No other dye was injected. The upstream boundary conditions for temperature, BOD, and dissolved oxygen were constant at 10°C, 8 mg/L, and 9 mg/L, respectively.

This Appendix shows the utility of the TDDS. If OXYGEN.F77 is to be used without the TDDS, only a couple of characters in the file need to be changed according to instructions within the code. The remainder of this Appendix contains the format for OXYGEN.INPUT, the input files LTM.INPUT and OXYGEN.INPUT, and the output file OXYGEN.OUTPUT.

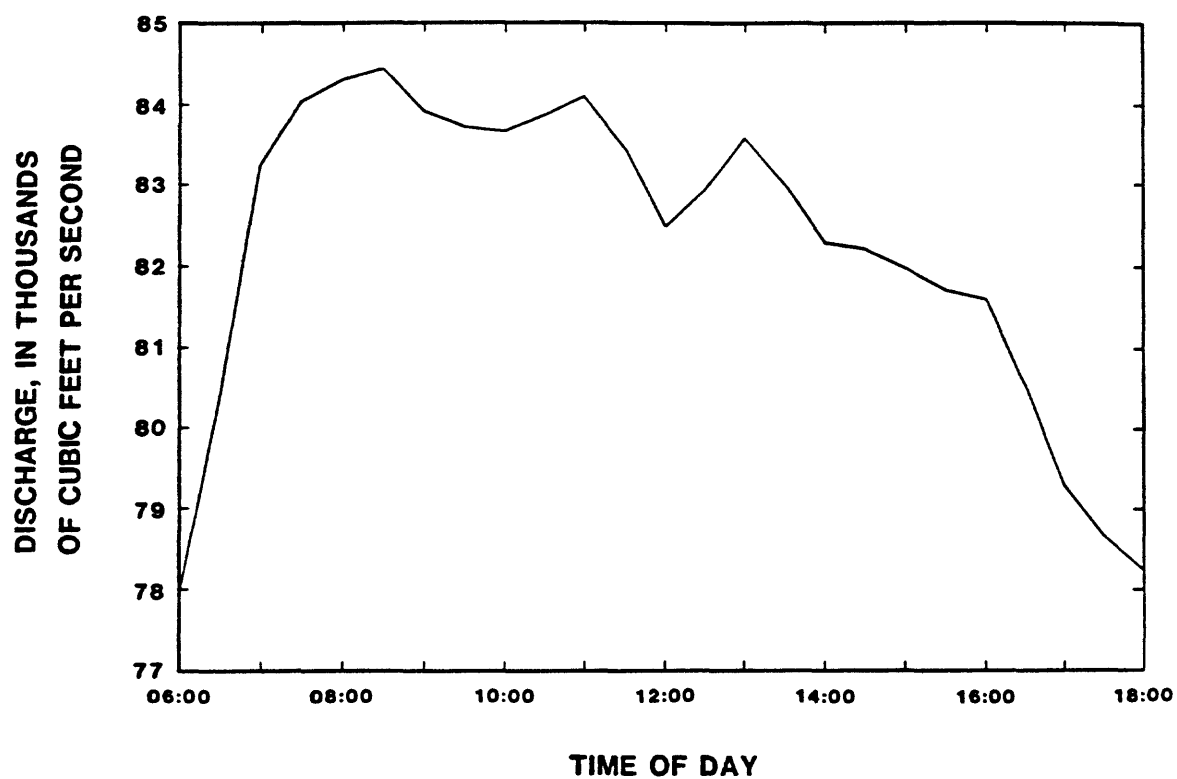


Figure 8.--Ohio River discharge at Greenup Dam, April 19, 1978.

 Data Set 1 -- OXYGEN.F77 Coefficient Card

ALWAYS REQUIRED

Field	Variable	Format	Description
0		10X	Card label
1	CK1	F7.0	BOD decay coefficient, (1/day)
2	CK2	F7.0	Reaeration coefficient, (1/day)
3	CK4	F7.0	Benthos source rate for BOD (1/day)
4	A1	F7.0	Evaporation in millimeters per day per kilopascal of vapor gradient (mm per day per kpa)
5	B1	F7.0	Evaporation in millimeters per day per m/sec of windspeed and kilopascal of vapor gradient (mm/day per m/sec per kpa)
6-10			Empty

 Data Set 2 -- Temperature and Windspeeds

Include if the TDDS is not used

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	TA	F7.0	Air or equilibrium temperature during the first time step (Celsius)
2	V	F7.0	Windspeed during the first time step (m/sec)
3-10			Empty

**Repeat Data Set 2 for every time step (NTS times).

 LTM.INPUT

OHIO RIVER OXYGEN EXAMPLE										
SETUP CARD	8	0	0	77850.	6.0	48	0.25	-1	4	0
OUTPUT CRD	24	8	-1	0	1					
COF OUTPUT	24	6								
LABEL CARD	DYE	TEMP	BOD	DO						
RIVR MILES	13.8	12.2	10.2	8.2	6.2	4.2	2.2	0.0		
DQO	0.34	0.34	0.34	0.34	0.34	0.34	0.34	0.34		
INITIAL DI	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0		
INITIAL TM	10.0	9.0	8.0	7.0	6.0	5.0	5.0	5.0		
INITIAL BD	8.0	8.0	8.0	8.0	8.0	8.0	8.0	8.0		
INITIAL DO	9.0	9.0	9.0	9.0	9.0	9.0	9.0	9.0		
TDDS CONTR	10	0	1							
TDDS DATES	78	4	19	6	0	78	4	19	18	0
TDDS ST ID		3216600		3216601		3216602		3216900		3216901
TDDS ST ID		3216902		3216903		3217200				
TDDS INPUT	Q	48								
TDDS INPUT	A	48								
TDDS INPUT	B	48								
TDDS INPUT	C1	96	1	1						
TDDS INPUT	M1	96	1	8						
TDDS INPUT	C2	48	1	1						
TDDS INPUT	C3	48	1	1						
TDDS INPUT	C4	48	1	1						
TDDS INPUT	AT	48	1	1						
TDDS INPUT	WS	48	1	1						

 OXYGEN.INPUT

CK1,CK2 CD	1.0	10.0	600.0	3.01	1.13
------------	-----	------	-------	------	------

OHIO RIVER OXYGEN EXAMPLE

SIMULATION IS OF UNSTEADY FLOW
INPUT DATA IS ENGLISH
MODEL IS TO RUN 48 TIME STEPS EACH 0.25 HOURS LONG.
THE SIMULATION STARTS 6.0000 HOURS AFTER MIDNIGHT.
THE RIVER IS DISCRETIZED BY 8 GRID POINTS.
THE INITIAL UPSTREAM DISCHARGE IS CONSTANT AT 77850.00 CUBIC METERS OR FEET PER SEC.
EVERY 24 TIME STEPS DATA WILL BE PRINTED FOR THE FOLLOWING GRIDS:
1 2 3 4 5 6 7 8

THE CONSTITUENTS MODELED ARE:

1 OYE
2 TEMP
3 BOD
4 DO

DIRECTORY OF TIME-DEPENDENT DATA SETS IN DIRECT ACCESS FILE

PROCESSED BY PROGRAM "OADIO" ; VERSION 83/01/28

* * * *

PROCESSING DATE 85/ 4/ 1

DATA SET NO	FIELD STATION NUMBER	START OF ENTRY YR MO DY HR MN	END OF ENTRY YR MO DY HR MN	PROCESSING TIME YR MO DY HR MN	RDS PER DAY	DATA SET SIZE	TYPE OF DATA	FILE ADDRESS RECORD BYTE	DATA FLAGGED
1	3-2166.00	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	A	15 1137	NO
2	3-2166.00	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	B	15 2477	NO
3	3-2166.00	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	Q	14 6029	NO
4	3-2166.00	74/ 1/10 1: C	74/ 1/17 24: C	84/ 3/15 9:44	24	192	Z	8 2665	NO
5	3-2166.00	74/ 4/26 1: C	74/ 5/ 2 24: C	84/ 3/14 13:27	24	168	Z	7 1	NO
6	3-2166.00	74/ 6/ 1 1: C	74/ 6/ 8 24: C	84/ 3/14 13:27	24	192	Z	7 673	NO
7	3-2166.00	74/12/14 1: C	74/12/20 24: C	84/ 3/14 13:27	24	168	Z	7 1441	NO
8	3-2166.00	75/ 2/17 1: C	75/ 2/20 12: C	84/ 3/14 13:27	24	84	Z	7 2113	NO
9	3-2166.00	75/ 2/24 1: C	75/ 3/ 2 24: C	84/ 3/14 13:27	24	168	Z	7 2449	NO
10	3-2166.00	76/ 3/15 1: C	76/ 3/21 24: C	84/ 3/15 9:44	24	168	Z	8 3433	NO
11	3-2166.00	77/ 4/ 2 1: C	77/ 4/ 7 24: C	84/ 3/14 13:27	24	144	Z	7 3121	NO
12	3-2166.00	77/10/10 1: C	77/10/16 24: C	84/ 3/14 13:27	24	168	Z	7 3697	NO
13	3-2166.00	78/ 3/12 1: C	78/ 3/19 24: C	84/ 3/14 13:27	24	192	Z	7 4369	NO
14	3-2166.00	78/ 4/16 1: C	78/ 4/22 24: C	84/ 3/14 13:27	24	168	Z	7 5137	NO
15	3-2166.00	78/ 8/19 1: C	78/ 8/25 24: C	84/ 3/14 13:27	24	168	Z	7 5809	NO
16	3-2166.00	78/10/15 1: C	78/10/21 24: C	84/ 3/15 8:29	24	168	Z	8 249	NO
17	3-2166.00	78/11/11 1: C	78/11/17 24: C	84/ 3/15 8:29	24	168	Z	8 921	NO
18	3-2166.00	79/ 1/21 1: C	79/ 1/27 24: C	84/ 3/15 8:29	24	168	Z	8 1593	NO
19	3-2166.00	79/ 9/11 1: C	79/ 9/15 8: C	84/ 3/15 10:39	24	104	Z	8 4105	NO
20	3-2166.00	82/10/ 8 10: C	82/11/ 4 11: C	84/ 3/20 8:45	24	650	Z	8 4313	NO
21	3-2166.00	82/11/ 4 12: C	82/12/ 6 15: C	84/ 3/22 10:42	24	772	Z	8 5613	NO
22	3-2166.00	82/12/ 6 16: C	83/ 1/15 16: C	84/ 3/28 13:23	24	961	Z	13 2677	NO
23	3-2166.00	83/ 1/17 17: C	83/ 2/15 11: C	84/ 3/22 13:19	24	691	Z	9 2943	NO
24	3-2166.00	83/ 2/15 13: C	83/ 4/ 4 15: C	84/ 3/22 13:19	24	1155	Z	9 4325	NO
25	3-2166.00	83/ 4/ 4 17: C	83/ 5/17 14: C	84/ 3/22 13:19	24	1030	Z	10 403	NO
26	3-2166.00	83/ 5/17 20: C	83/ 6/29 17: C	84/ 3/22 13:19	24	1030	Z	10 2463	NO
27	3-2166.00	78/ 4/19 6: C	78/ 4/19 18: C	84/11/ 1 10:42	48	25	AT	20 1441	NO
28	3-2166.00	78/ 4/19 6: C	78/ 4/19 18: C	85/ 3/ 4 11:50	96	49	C1	20 1641	NO
29	3-2166.00	78/ 4/19 6: C	78/ 4/19 18: C	85/ 3/ 4 12:51	48	25	C2	20 1887	NO
30	3-2166.00	78/ 4/19 6: C	78/ 4/19 18: C	85/ 3/ 4 11:50	48	25	C3	20 1541	NO
31	3-2166.00	78/ 4/19 6: C	78/ 4/19 18: C	85/ 3/ 4 11:50	48	25	C4	20 1591	NO
32	3-2166.00	78/ 4/19 6: C	78/ 4/19 18: C	84/11/ 1 10:42	48	25	WS	20 1491	NO
33	3-2166.01	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	A	15 5157	NO
34	3-2166.01	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	B	16 265	NO
35	3-2166.01	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	Q	15 3817	NO
36	3-2166.02	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	A	16 2945	NO
37	3-2166.02	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	B	16 4285	NO
38	3-2166.02	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	Q	16 1605	NO
39	3-2166.00	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	A	17 733	NO
40	3-2166.00	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	B	17 2073	NO
41	3-2166.00	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	Q	16 5625	NO
42	3-2166.01	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	A	17 4753	NO
43	3-2166.01	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	B	17 6093	NO
44	3-2166.01	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	Q	17 3413	NO
45	3-2166.02	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	A	18 2541	NO
46	3-2166.02	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	B	18 3881	NO
47	3-2166.02	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	Q	18 1201	NO
48	3-2166.03	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	A	19 329	NO
49	3-2166.03	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	B	19 1669	NO
50	3-2166.03	78/ 4/16 1: C	78/ 4/22 24: C	84/10/26 14:26	48	335	Q	18 5221	NO

DATA SET NO	FIELD STATION NUMBER	START OF ENTRY YR MO DY HR MN	END OF ENTRY YR MO DY HR MN	PROCESSING TIME YR MO DY HR MN	RDS PER DAY	DATA SET SIZE	TYPE OF DATA	FILE ADDRESS RECORD BYTE	DATA FLAGGED
51	3-2172.00	78/ 4/16 1: C	78/ 4/22 24: O	84/10/26 14:26	48	335	A	19 4349	NO
52	3-2172.00	78/ 4/16 1: O	78/ 4/22 24: O	84/10/26 14:26	48	335	B	19 5689	NO
53	3-2172.00	78/ 4/16 1: O	78/ 4/22 24: C	84/10/26 14:26	48	335	Q	19 3009	NO
54	3-2172.00	82/12/ 6 16: C	83/ 1/15 13: O	84/ 4/ 6 12:27	48	1915	Q	13 4601	NO
55	3-2172.00	74/ 1/10 1: C	74/ 1/17 24: O	84/ 3/15 9:44	24	192	Z	8 3049	NO
56	3-2172.00	74/ 4/26 1: C	74/ 5/ 2 24: O	84/ 3/14 13:27	24	168	Z	7 337	NO
57	3-2172.00	74/ 6/ 1 1: O	74/ 6/ 8 24: O	84/ 3/14 13:27	24	192	Z	7 1057	NO
58	3-2172.00	74/12/14 1: O	74/12/20 24: O	84/ 3/14 13:27	24	168	Z	7 1777	NO
59	3-2172.00	75/ 2/17 1: O	75/ 2/20 12: O	84/ 3/14 13:27	24	84	Z	7 2281	NO
60	3-2172.00	75/ 2/24 1: O	75/ 3/ 2 24: O	84/ 3/14 13:27	24	168	Z	7 2785	NO
61	3-2172.00	76/ 3/15 1: C	76/ 3/21 24: O	84/ 3/15 9:44	24	168	Z	8 3769	NO
62	3-2172.00	77/ 4/ 2 1: O	77/ 4/ 7 24: O	84/ 3/14 13:27	24	144	Z	7 3409	NO
63	3-2172.00	77/10/10 1: O	77/10/16 24: O	84/ 3/14 13:27	24	168	Z	7 4033	NO
64	3-2172.00	78/ 3/12 1: C	78/ 3/19 24: O	84/ 3/14 13:27	24	192	Z	7 4753	NO
65	3-2172.00	78/ 4/16 1: O	78/ 4/22 24: O	84/ 3/14 13:27	24	168	Z	7 5473	NO
66	3-2172.00	78/ 8/19 1: C	78/ 8/25 24: C	84/ 3/28 8:46	24	168	Z	12 4733	NO
67	3-2172.00	78/10/15 1: O	78/10/21 24: O	84/ 3/15 8:29	24	168	Z	8 585	NO
68	3-2172.00	78/11/11 1: O	78/11/17 24: O	84/ 3/15 8:29	24	168	Z	8 1257	NO
69	3-2172.00	79/ 1/21 1: C	79/ 1/27 24: O	84/ 3/15 8:29	24	168	Z	8 1929	NO
70	3-2172.00	79/ 9/11 1: O	79/ 9/15 8: O	84/ 3/15 9:44	24	104	Z	8 2457	NO
71	3-2172.00	82/10/ 8 10: C	82/11/ 4 10: O	84/ 3/22 13:19	24	649	Z	10 4523	NO
72	3-2172.00	82/11/ 4 12: O	82/12/ 6 14: O	84/ 3/22 13:19	24	771	Z	10 5821	NO
73	3-2172.00	82/12/ 6 15: O	83/ 1/15 13: O	84/ 3/28 12: 3	24	959	Z	13 759	NO
74	3-2172.00	83/ 1/17 17: O	83/ 2/15 12: O	84/ 3/22 13:19	24	692	Z	11 3145	NO
75	3-2172.00	83/ 2/15 13: O	83/ 4/ 4 15: O	84/ 3/22 13:19	24	1155	Z	11 4529	NO
76	3-2172.00	83/ 4/ 4 17: C	83/ 5/17 18: O	84/ 3/22 13:19	24	1034	Z	12 607	NO
77	3-2172.00	83/ 5/17 20: C	83/ 6/29 16: O	84/ 3/22 13:19	24	1029	Z	12 2675	NO
78	3-2172.00	78/ 4/19 6: O	78/ 4/19 18: O	85/ 3/ 4 11:50	96	49	M1	20 1789	NO

INITIAL CONDITIONS

GRID	RIVER KM	TRIB. FLOW CU M/SEC	VELOCITY M/HR	AREA SQ M	TOP WIDTH METERS	LAT FLOW SQ M/S	DISP FACT DQQ	INITIAL CONCENTRATIONS OF CONSTITUENTS			
								1	2	3	4
1	22.21	0.000	2829.9	2804.38	468.68	0.000000	0.34	0.0	10.0	8.0	9.0
2	19.63	0.000	3011.4	2635.32	530.94	0.000000	0.34	0.0	9.0	8.0	9.0
3	16.42	0.000	3739.1	2122.47	447.40	0.000000	0.34	0.0	8.0	8.0	9.0
4	13.20	0.000	3917.6	2025.74	397.16	0.000000	0.34	0.0	7.0	8.0	9.0
5	9.98	0.000	3543.3	2239.72	399.52	0.000000	0.34	0.0	6.0	8.0	9.0
6	6.76	0.000	3577.9	2218.10	417.62	0.000000	0.34	0.0	5.0	8.0	9.0
7	3.54	0.000	3298.3	2035.76	418.80	0.000000	0.34	0.0	5.0	8.0	9.0
8	-0.00	0.000						0.0	5.0	8.0	9.0

TIME DAY	HOOR	GRID NUMBER	TRAVEL TIME(HR)	CONSTI TUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			
							DECAY	DISP	LATE	TRIB
1	12.00	1	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.00	10.00	0.00	0.00	0.00	0.00
				BCD	8.00	8.00	0.00	0.00	0.00	0.00
				DO	9.00	9.00	0.00	0.00	0.00	0.00
		2	0.28	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.04	10.00	0.03	0.00	0.00	0.00
				BCD	7.82	8.00	-0.16	-0.02	0.00	0.00
				DO	9.43	9.00	0.38	0.05	0.00	0.00
		3	1.53	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.08	10.00	0.07	0.00	0.00	0.00
				BCD	7.62	8.00	-0.36	-0.02	0.00	0.00
				DO	9.78	9.00	0.76	0.03	0.00	0.00
		4	2.77	DYE	0.07	0.00	0.00	0.07	0.00	0.00
				TEMP	10.10	10.00	0.10	-0.00	0.00	0.00
				BCD	7.43	8.00	-0.56	-0.02	0.00	0.00
				DO	10.04	9.00	1.02	0.02	0.00	0.00
		5	3.57	DYE	0.52	0.00	0.00	0.52	0.00	0.00
				TEMP	10.10	10.00	0.11	-0.01	0.00	0.00
				BCD	7.22	8.00	-0.70	-0.02	0.00	0.00
				DO	10.15	9.00	1.18	0.02	0.00	0.00
		6	4.45	DYE	1.26	0.00	0.00	1.26	0.00	0.00
				TEMP	10.07	10.00	0.10	-0.03	0.00	0.00
				BCD	7.14	8.00	-0.85	-0.01	0.00	0.00
				DO	10.31	9.00	1.30	0.01	0.00	0.00

CR(I1,I2)

I2	I1			
	1	2	3	4
1	0.000	0.000	0.000	0.000
2	0.000	17.000	0.000	0.000
3	0.000	0.000	0.000	0.000
4	0.000	0.000	0.000	11.230

XK(I1,I2)

I2	I1			
	1	2	3	4
1	0.000	0.000	0.000	0.000
2	0.000	-0.008	0.000	0.000
3	0.000	0.000	-0.026	-0.026
4	0.000	0.000	0.000	-0.356

S(I1)

I1			
1	2	3	4
0.000	0.000	0.000	-0.000

TIME		GRID NUMBER	TRAVEL TIME(HR)	CONSTI TUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			TC TRIB
DAY	HOOR						DECAY	DISP	LATC	
1	18.00	7	5.34	DYE	3.82	9.67	0.00	-5.85	0.00	0.00
				TEMP	9.91	10.00	0.09	-0.18	0.00	0.00
				BOD	6.99	8.00	-1.03	0.02	0.00	0.00
				DO	10.46	9.00	1.46	0.01	0.00	0.00
		8	0.00	DYE	2.85	0.00	0.00	2.85	0.00	0.00
				TEMP	9.45	9.59	0.09	-0.23	0.00	0.00
				BOD	6.91	8.00	-1.15	0.06	0.00	0.00
				DO	10.64	9.00	1.68	-0.04	0.00	0.00
		1	0.00	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.00	10.00	0.00	0.00	0.00	0.00
				BOD	8.00	8.00	0.00	0.00	0.00	0.00
				DO	9.00	9.00	0.00	0.00	0.00	0.00
		2	0.94	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.02	10.00	0.02	0.00	0.00	0.00
				BOD	7.82	8.00	-0.16	-0.02	0.00	0.00
				DO	9.43	9.00	0.38	0.05	0.00	0.00
		3	2.03	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.08	10.00	0.07	0.01	0.00	0.00
				BOD	7.57	8.00	-0.41	-0.02	0.00	0.00
				DO	9.85	9.00	0.83	0.02	0.00	0.00
		4	2.91	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.14	10.00	0.12	0.01	0.00	0.00
				BOD	7.42	8.00	-0.56	-0.02	0.00	0.00
				DO	10.04	9.00	1.02	0.02	0.00	0.00
		5	3.75	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.20	10.00	0.19	0.01	0.00	0.00
				BOD	7.28	8.00	-0.71	-0.02	0.00	0.00
				DO	10.17	9.00	1.16	0.01	0.00	0.00
		6	4.65	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.28	10.00	0.28	0.00	0.00	0.00
				BOD	7.09	8.00	-0.90	-0.02	0.00	0.00
				DO	10.31	9.00	1.30	0.01	0.00	0.00
		7	5.55	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.35	10.00	0.36	-0.00	0.00	0.00
				BOD	6.90	8.00	-1.09	-0.02	0.00	0.00
				DO	10.40	9.00	1.39	0.01	0.00	0.00
		8	6.48	DYE	0.00	0.00	0.00	0.00	0.00	0.00
				TEMP	10.40	10.00	0.40	-0.01	0.00	0.00
				BOD	6.76	8.00	-1.22	-0.01	0.00	0.00
				DO	10.45	9.00	1.45	0.01	0.00	0.00
CONSTITUENT		RMS ERROR								
DYE		0.00587								

APPENDIX H

QUAL II REACTION KINETICS

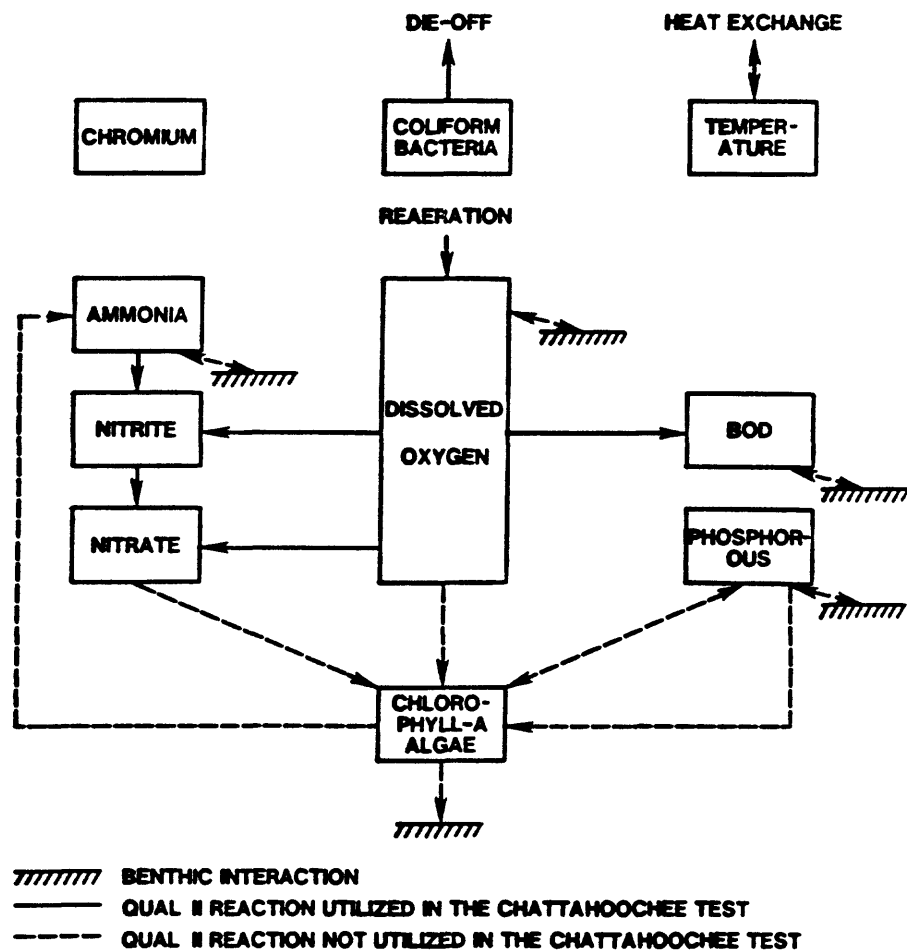
Schoellhamer (in press) showed that the reaction kinetics of the SEMCOG version of QUAL II, a popular one-dimensional Eulerian water-quality model (Roesner and others, 1977a and 1977b), can be inserted into the LTM to form a hybrid water-quality model. For an equally posed problem the hybrid model mimics the QUAL II model, but the LTM can model unsteady constituent loads and unsteady flows with the advantage of Lagrangian calculations while QUAL II can only model steady loads and steady flow. An example of a steady state application of the hybrid model to the Chattahoochee River in Georgia is presented in this Appendix. McCutcheon (1983) and Schoellhamer (in press) give more information on the data set and Schoellhamer (in press) gives more information on the testing of the hybrid model.

This Appendix lists LTM.INPUT, the decay-coefficient subroutine input file QUAL2.INPUT, and output file QUAL2.OUTPUT, and the format for QUAL2.INPUT. The LTM Programmers Manual lists the decay-coefficient subroutine QUAL2.F77 (Schoellhamer and Jobson, 1986).

The QUAL II reaction kinetics are discussed in detail by Roesner and others (1977a and 1977b). Figure 9 shows a schematic diagram of the QUAL II kinetics. The constituents included in the hybrid model are temperature, algae, ammonia, nitrite, nitrate, orthophosphate, biochemical oxygen demand, dissolved oxygen, coliform, and an arbitrary nonconservative constituent. Temperature is presently modeled by the QUAL II temperature algorithm, but QUAL2.F77 contains instructions on how to replace that algorithm with Jobson's (1981) simplified temperature algorithm. Although McCutcheon (1983) satisfactorily modeled water quality in several rivers with the QUAL II kinetics, the user is responsible for determining if these kinetics are applicable to a specific modeling task. If the kinetics are unsatisfactory, the LTM Programmers Manual allows a user to easily code and apply any desired set of reaction kinetics.

Load the program with the compiled LTM.F77 and QUAL2.F77.

The file LTM.INPUT for the May/June 1977 Chattahoochee River test is listed in this Appendix. The 79 kilometer study reach of the Chattahoochee River contains 25 grid points with 23 point sources and sinks. 190 0.25 hour time steps are used because the travel time through the reach of 43.56 hours has to be exceeded in order to establish a completely steady state solution. Thus at the end of the simulation, all of the parcels initially located in the river were flushed out of the system. In order to establish a completely steady state solution and to pose the same problem to the LTM as was originally posed to the QUAL II model, the boundary conditions were held constant. Only the boundary conditions during the first time step are



QUAL II CONSTITUENTS AND REACTIONS

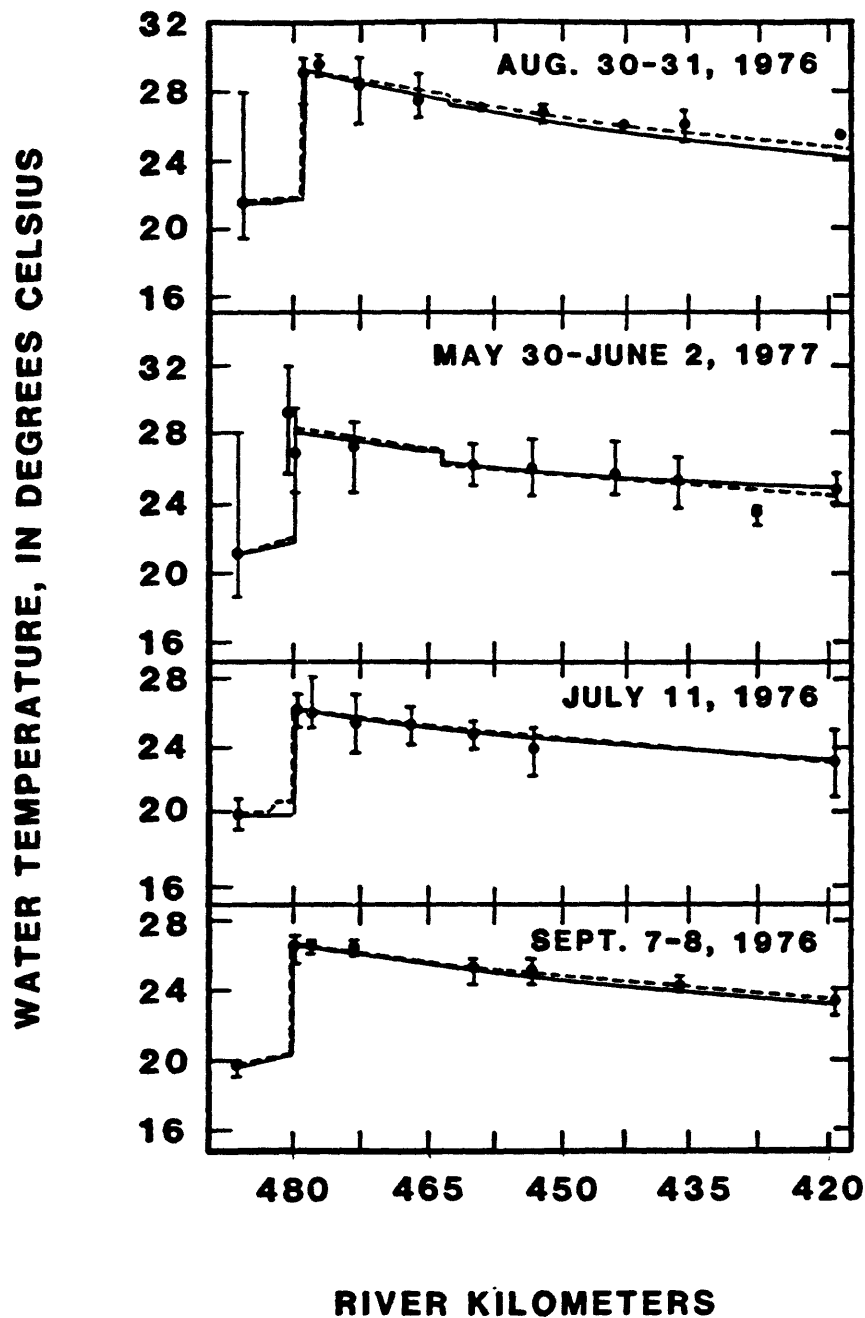
Figure 9.--QUAL II constituents and reactions.

included in the list of LTM.INPUT in this Appendix but the actual file contains 190 repetitions of the boundary conditions. Because the solution does not vary with time, output is written at the last time step only. The DQQ of 0.0036 was calculated from equation 12 with the longitudinal dispersion coefficient calculated by QUAL II. The time step was not decreased to increase DQQ because the 0.25 hour time step produced a number of parcels nearly equal to the number of QUAL II computational elements which was needed for a fair comparison of the two models. The dispersion in this example is very low because the dispersion coefficient calculated by QUAL II is very low for a natural river.

The results of this run are effectively identical to the equivalent QUAL II run. Temperature results for this and three other data sets are shown in Figure 10. This Figure also shows that the simplified temperature model satisfactorily models temperature.

Jobson (1984) used an earlier version of the LTM to model unsteady conditions in the Chattahoochee River. This data was used by Schoellhamer (in press) to show the importance of considering unsteady phenomenon.

This Appendix presents the LTM/QUAL II hybrid water-quality model that gives the user the advantages of Lagrangian calculations and the QUAL II reaction kinetics. The remainder of this Appendix contains the format for QUAL2.INPUT, the input files LTM.INPUT and QUAL2.INPUT, and the output file QUAL2.OUTPUT.



I Mean and Range of Observations
 — QUAL II and LTM Hybrid Model
 - - - LTM Simplified Temperature Model

Figure 10.--Observed and predicted water temperatures in the Chattahoochee River, Georgia.

 Data Set 1 -- Number of Reaches Card

Field	Variable	Format	Description
0		10X	Card label
1	INX	I7	Number of reaches in simulation, equal to NXSEC-1
2	DT	F7.0	Simulation time step (hours), REQUIRED ONLY IF FUNCTION HSNET IS BEING USED
3-10			Empty

 Data Set 2 -- ALPHA0 Coefficients

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	ALPHA0(1)	F7.0	Ratio of chlorophyll-a to algae biomass in reach 1 (ug Chl-a/mg A)
2	ALPHA0(2)	F7.0	Ratio of chlorophyll-a to algae biomass in reach 2 (ug Chl-a/mg A)
.	.	.	.
:	:	:	:
.	.	.	.
INX	ALPHA0(INX)	F7.0	Ratio of chlorophyll-a to algae biomass in reach INX (ug Chl-a/mg A)

Data Set 3 -- ALPHA and Algae Coefficients Card

Field	Variable	Format	Description
0		10X	Card label
1	ALPHA(1)	F7.0	Fraction of algae biomass which is N (mg N/mg A)
2	ALPHA(2)	F7.0	Fraction of algae biomass which is P (mg P/mg A)
3	ALPHA(3)	F7.0	Oxygen production per unit of algae growth (mg O/mg A)
4	ALPHA(4)	F7.0	Oxygen uptake per unit of algae respired (mg O/mg A)
5	ALPHA(5)	F7.0	Oxygen uptake per unit of ammonia oxidation (mg O/mg N)
6	ALPHA(6)	F7.0	Oxygen uptake per unit of nitrite oxidation (mg O/mg N)
7	GROMAX	F7.0	Maximum specific growth rate of algae (1/day)
8	RESPRT	F7.0	Algae respiration rate (1/day)
9-10			Empty

 Data Set 4 -- CKNH3 Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CKNH3(1)	F7.0	Rate constant for biological oxidation of ammonia to nitrite in reach 1 (1/day)
2	CKNH3(2)	F7.0	Rate constant for biological oxidation of ammonia to nitrite in reach 2 (1/day)
.	.	.	.
:	:	:	:
.	.	.	.
INX	CKNH3(INX)	F7.0	Rate constant for biological oxidation of ammonia to nitrite in reach INX (1/day)

 Data Set 5 -- CKNO2 Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CKNO2(1)	F7.0	Rate constant for biological oxidation of nitrite to nitrate in reach 1 (1/day)
2	CKNO2(2)	F7.0	Rate constant for biological oxidation of nitrite to nitrate in reach 2 (1/day)
.	.	.	.
:	:	:	:
.	.	.	.
INX	CKNO2(INX)	F7.0	Rate constant for biological oxidation of nitrite to nitrate in reach INX (1/day)

 Data Set 6 -- ALGSET Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	ALGSET(1)	F7.0	Local settling rate for algae in reach 1 (ft/day)
2	ALGSET(2)	F7.0	Local settling rate for algae in reach 2 (ft/day)
.	.	.	.
.	.	.	.
.	.	.	.
INX	ALGSET(INX)	F7.0	Local settling rate for algae in reach INX (ft/day)

 Data Set 7 -- SPHOS Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	SPHOS(1)	F7.0	Benthos source rate for phosphorous in reach 1 (mg P/day-ft)
2	SPHOS(2)	F7.0	Benthos source rate for phosphorous in reach 2 (mg P/day-ft)
.	.	.	.
.	.	.	.
.	.	.	.
INX	SPHOS(INX)	F7.0	Benthos source rate for phosphorous in reach INX (mg P/day-ft)

 Data Set 8 -- SNH3 Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	SNH3(1)	F7.0	Benthos source rate for ammonia in reach 1 (mg N/day-ft)
2	SNH3(2)	F7.0	Benthos source rate for ammonia in reach 2 (mg N/day-ft)
.	.	.	.
.	.	.	.
.	.	.	.
INX	SNH3(INX)	F7.0	Benthos source rate for ammonia in reach INX (mg N/day-ft)

 Data Set 9 -- CK1 Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CK(1,1)	F7.0	Carbonaceous BOD decay rate in reach 1 (1/day)
2	CK(2,1)	F7.0	Carbonaceous BOD decay rate in reach 2 (1/day)
.	.	.	.
.	.	.	.
.	.	.	.
INX	CK(INX,1)	F7.0	Carbonaceous BOD decay rate in reach INX (1/day)

 Data Set 10 -- CK2 Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CK(1,2)	F7.0	Reaeration rate in reach 1 (1/day)
2	CK(2,2)	F7.0	Reaeration rate in reach 2 (1/day)
.	.	.	.
.	.	.	.
INX	CK(INX,2)	F7.0	Reaeration rate in reach INX (1/day)

 Data Set 11 -- CK3 Values

Reach	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CK(1,3)	F7.0	Carbonaceous BOD sink rate in reach 1 (1/day)
2	CK(2,3)	F7.0	Carbonaceous BOD sink rate in reach 2 (1/day)
.	.	.	.
.	.	.	.
.	.	.	.
INX	CK(INX,3)	F7.0	Carbonaceous BOD sink rate in reach INX (1/day)

 Data Set 12 -- CK4 Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CK(1,4)	F7.0	Benthos source rate for BOD in reach 1 (mg/day-ft)
2	CK(2,4)	F7.0	Benthos source rate for BOD in reach 2 (mg/day-ft)
.	.	.	.
:	:	:	:
.	.	.	.
INX	CK(INX,4)	F7.0	Benthos source rate for BOD in reach INX (mg/day-ft)

 Data Set 13 -- CK5 Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CK(1,5)	F7.0	Coliform die-off rate in reach 1 (1/day)
2	CK(2,5)	F7.0	Coliform die-off rate in reach 2 (1/day)
.	.	.	.
:	:	:	:
.	.	.	.
INX	CK(INX,5)	F7.0	Coliform die-off rate in reach INX (1/day)

 Data Set 14 -- CK6 Values

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CK(1,6)	F7.0	Arbitrary nonconservative decay rate in reach 1 (1/day)
2	CK(2,6)	F7.0	Arbitrary nonconservative decay rate in reach 2 (1/day)
.	.	.	.
.	.	.	.
.	.	.	.
INX	CK(INX,6)	F7.0	Arbitrary nonconservative decay rate in reach INX (1/day)

 Data Set 15 -- Coefficients Card

Field	Variable	Format	Description
0		10X	Card label
1	CKN	F7.0	Nitrogen half-saturation constant for algae growth (mg/l)
2	CKP	F7.0	Phosphorous half-saturation constant for algae growth (mg/l)
3	CKL	F7.0	Light half-saturation constant for algae growth (Langleys/min)
4	EXCOEF	F7.0	Light extinction coefficient (1/meter)
5-10			Empty

Data Set 16 -- Climatological Data

Include if the simplified temperature algorithm is used

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	SONET	F7.0	Net solar radiation during the first time step (Langleys/min)
2	TA	F7.0	Atmospheric or equilibrium temperature during the first time step (Celsius)
3	V	F7.0	Windspeed during the first time step (m/sec)
4-10			Empty

**Repeat this data set for every time step (NTS times)

 Data Set 17 -- Net Solar Radiation Algorithm Card

Include if the QUAL II temperature algorithm is used

Field	Variable	Format	Description
0		10X	Card label
1	JDAT	I7	Starting Julian date (1,...,365,366(?))
2	LAT	F7.0	Mean latitude of river basin (degrees)
3	LLM	F7.0	Local meridian of river basin (degrees)
4	LSM	F7.0	Standard meridian of time zone in which river basin is located (degrees)
5	ELEV	F7.0	Mean elevation of river basin (feet)
6	DAT	F7.0	Dust attenuation coefficient
7	AE	F7.0	Evaporation coefficient (ft/hour-in Hg)
8	BE	F7.0	Evaporation coefficient (ft/hour-in Hg-mi/h)
9-10			Empty

 Data Set 18 -- Climatological Data

Include if the QUAL II temperature algorithm is used

Field	Variable	Format	Description
0		10X	Card label, on all cards in data set
1	CLOUD	F7.0	Fraction of cloud cover ($0 \leq \text{CLOUD} \leq 1$)
2	DRYBLB	F7.0	Dry bulb temperature (degrees F or C)
3	WETBLB	F7.0	Wet bulb temperature (degrees F or C)
4	ATMPR	F7.0	Barometric pressure (in Hg or mb)
5	WIND	F7.0	Wind speed (ft/sec or m/sec)
6	METRIC	I7	Unit control for climatological data: -English units, METRIC = 0 -Metric units, METRIC <> 0
7	ISTDY	I7	Steady state climate control: -Steady state climate simulation, ISTDY = 1 -Unsteady climate simulation, ISTDY = 0
8-10			Empty

**If ISTDY = 0, repeat this data set once every three hours of simulation time.

QUAL2 FINK, MAY-JUNE 1977 CHATAHOOCHEE DATA											
SETUP CARD	25	23	0	31.72	7.30	190	0.25	0	8	1	
WRITE CARD	190	4	0	0	1						
OUTPUT GRD	1	7	8	25							
COEFF CARD	190	1									
LABEL CARD	TEMP(C)	ALGAE	AMMONIA	NITRITEN	NITRATE	PHOSPT	BOD	DISS	0		
RIVER KILO	487.58	483.80	483.70	483.64	483.19	481.76	481.42	478.78	474.96	473.60	
RIVER KILO	469.28	469.24	464.42	456.70	456.31	455.88	452.98	446.43	444.10	441.75	
RIVER KILO	440.09	430.24	421.20	420.44	418.19						
AREAS CARD	102.2	102.2	102.2	89.9	89.9	161.3	91.0	91.0	80.7	71.9	
AREAS CARD	104.7	82.1	82.1	143.8	95.4	97.0	120.0	106.4	115.5	131.4	
AREAS CARD	112.7	123.6	58.7	121.7	105.8						
TOPWD CARD	78.4	78.4	78.4	68.1	68.1	125.3	59.7	59.7	73.0	29.8	
TOPWD CARD	82.5	58.5	58.5	86.5	67.5	56.6	83.9	63.1	78.3	78.4	
TOPWD CARD	81.2	66.2	47.6	70.8	69.3						
TRIBS CARD	2	0.00	3	0.37	4	2.46	5	4.25	6	-10.02	
TRIBS CARD	7	10.02	8	0.21	9	0.59	10	0.42	11	0.541	
TRIBS CARD	12	0.37	13	0.06	14	0.25	15	0.54	16	0.59	
TRIBS CARD	17	0.74	18	0.74	19	0.57	20	0.45	21	1.87	
TRIBS CARD	22	0.58	23	1.16	24	0.85					
DQQ VALUES	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	
DQQ VALUES	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	
DQQ VALUES	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	.00336	
INIT COND1	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	
INIT COND1	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	
INIT COND1	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	
INIT COND2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
INIT COND2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
INIT COND2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
INIT COND3	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	
INIT COND3	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	
INIT COND3	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	
INIT COND4	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	
INIT COND4	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	
INIT COND4	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	
INIT COND5	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	
INIT COND5	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	
INIT COND5	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	
INIT COND6	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	
INIT COND6	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	
INIT COND6	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	
INIT COND7	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	
INIT COND7	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	
INIT COND7	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	
INIT COND8	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	
INIT COND8	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	
INIT COND8	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	
BC TEMP C1	21.6	21.1	21.5	22.3	23.8	27.2	46.7	21.7	21.5	20.6666	
BC TEMP C2	22.0	26.6	21.7	22.0	21.4	20.1	20.6	20.6	20.3	21.666	
BC TEMP C3	21.3	20.5	21.1	22.0							
BC ALGAE C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
BC ALGAE C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
BC ALGAE C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
BC AMMO C1	0.01	0.0	11.0	0.10	15.0	0.0	1.74	3.40	0.03	13.0	
BC AMMO C2	13.0	0.16	0.05	5.70	0.08	0.01	0.02	0.02	0.02	0.0011	
BC AMMO C3	0.02	0.03	0.18	0.06							
BC NTRI C1	0.05	0.00	0.05	0.02	0.01	0.00	0.04	0.04	0.01	0.08	
BC NTRI C2	0.01	0.02	0.01	0.08	0.03	0.01	0.01	0.01	0.01	0.01	
BC NTRI C3	0.01	0.00	0.01	0.01							
BC NTRA C1	0.24	0.00	0.28	0.43	0.00	0.00	0.25	0.28	0.67	0.04	
BC NTRA C2	0.01	0.40	0.28	0.70	0.67	0.45	0.44	0.44	0.18	0.36	
BC NTRA C3	0.23	0.18	0.01	0.21							
BC PHOS C1	0.01	0.00	2.90	0.04	3.10	0.00	0.38	0.00	0.02	6.00	
BC PHOS C2	3.10	0.05	0.00	5.10	0.11	0.10	0.06	0.06	0.01	0.03	
BC PHOS C3	0.01	0.00	0.00	0.01							
BC BOD C1	4.10	0.00	64.00	6.70	79.00	0.00	13.00	2.90	4.60	84.00	
BC BOD C2	29.00	5.70	5.10	11.00	4.40	4.40	4.00	4.00	4.30	3.60	
BC BOD C3	4.10	3.70	3.80	3.70							
BC DO C1	9.20	0.00	0.70	7.10	9.20	0.00	8.50	4.00	8.70	0.60	
BC DO C2	3.00	7.50	7.70	3.90	8.00	8.40	8.80	8.80	10.00	8.60	
BC DO C3	9.00	8.60	8.80	8.20							

**190 repetitions of the boundary conditions (BC cards) are in LTM.INPUT.

CROSS SECS	24	0.25									
ALPHA0 CRD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ALPHA0 CRD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ALPHA0 CRD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ALPHA+ CRD	0.08	0.012	1.6	2.0	3.43	1.14	1.0	0.2	0.0	0.0	0.0
CKNH3 CARD	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
CKNH3 CARD	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
CKNH3 CARD	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
CKNO2 CARD	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6
CKNO2 CARD	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6
CKNO2 CARD	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6
ALGSET CRD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ALGSET CRD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ALGSET CRD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SPHOS CARD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
SPHOS CARD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
SPHOS CARD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
SNH3 CARD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
SNH3 CARD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
SNH3 CARD	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
CK1 VALUES	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
CK1 VALUES	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
CK1 VALUES	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
CK2 VALUES	1.75	1.75	1.75	0.54	0.54	0.54	1.21	1.21	1.21	1.21	1.46
CK2 VALUES	1.03	1.03	1.03	0.84	0.84	0.84	0.29	0.57	0.98	0.98	0.98
CK2 VALUES	2.06	2.77	1.17	1.17							
CK3 VALUES	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
CK3 VALUES	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
CK3 VALUES	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
CK4 VALUES	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
CK4 VALUES	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
CK4 VALUES	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
CK5 VALUES	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08
CK5 VALUES	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08
CK5 VALUES	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08
CK6 VALUES	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.000
CK6 VALUES	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.000
CK6 VALUES	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.000
COEFF CARD	0.03	0.012	600.0	0.1							
TEMPS CARD	242	33.0	84.0	75.0	750.0	0.04	0.001	0.000163			
CLMAT CARD	0.60	74.5	64.5	29.85	10.8	0	1				

QUAL2 FINK, MAY-JUNE 1977 CHATAMCCCHEE DATA

SIMULATION IS OF STEADY FLOW
 INPUT DATA IS METRIC
 MODEL IS TO RUN 190 TIME STEPS EACH 0.25 HOURS LONG.
 THE SIMULATION STARTS 7.3000 HOURS AFTER MIDNIGHT.
 THE RIVER IS DISCRETIZED BY 25 GRID POINTS.
 THE INITIAL UPSTREAM DISCHARGE IS CONSTANT AT 31.72 CUBIC METERS OR FEET PER SEC.
 EVERY 190 TIME STEPS DATA WILL BE PRINTED FOR THE FOLLOWING GRIDS:
 1 7 8 25

THE CONSTITUENTS MODELED ARE:

1 TEMP(C)
 2 ALGAE
 3 AMMONIA
 4 NITRITE
 5 NITRATE
 6 PHOSPHY
 7 BOD
 8 DISS O

INITIAL CONDITIONS

GRID	RIVER KM	TRIB. FLOW CU M/SEC	VELOCITY M/HR	AREA SQ M	TCP WIDTH METERS	LAT FLOW SQ M/S	DISP FACT DQQ	INITIAL CONCENTRATIONS OF CONSTITUENTS							
								1	2	3	4	5	6	7	8
1	487.58	0.000	1117.3	102.20	78.40	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
2	483.80	0.000	1117.3	102.20	78.40	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
3	483.70	0.370	1202.7	96.05	73.25	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
4	483.64	2.460	1383.5	89.90	68.10	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
5	483.19	4.250	1112.1	125.60	96.70	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
6	481.76	-10.020	821.3	126.15	92.50	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
7	481.42	10.020	1534.9	91.00	59.70	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
8	478.78	0.210	1635.8	85.85	66.35	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
9	474.96	0.590	1868.4	76.30	51.40	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
10	473.60	0.420	1631.6	88.30	56.15	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
11	469.28	0.540	1563.3	93.40	70.50	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
12	469.24	0.370	1794.7	82.10	58.50	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
13	464.42	4.060	1457.7	112.95	72.50	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
14	456.70	0.250	1421.9	119.60	77.00	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
15	456.31	0.540	1788.0	96.20	62.05	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
16	455.88	0.590	1604.9	108.50	70.25	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
17	452.98	0.740	1561.8	113.20	73.50	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
18	446.43	0.740	1617.5	110.95	70.70	0.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0
19	444.10	0.570						25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0

Appendix H

QUAL II Reaction Kinetics

QUAL2.OUTPUT

20	441.75	C.45C	1470.3	123.45	78.35	C.000000	0.00	25.0	C.0	C.0	0.0	0.2	0.0	4.0	10.0
21	440.09	1.87C	1500.5	122.05	79.80	C.000000	0.00	25.0	C.0	0.0	0.0	0.2	C.0	4.0	10.0
22	430.24	C.58C	1607.0	118.15	73.70	C.000000	0.00	25.0	C.0	0.0	0.0	0.2	0.0	4.0	10.0
23	421.20	1.16C	2105.9	91.15	56.90	C.000000	0.00	25.0	C.0	0.0	0.0	0.2	0.0	4.0	10.0
24	420.44	C.85C	2174.4	90.2C	59.20	C.000000	0.00	25.0	C.0	0.0	0.0	0.2	0.0	4.0	10.0
25	418.19	C.00C	1751.1	113.75	70.05	C.000000	0.00	25.0	0.0	0.0	0.0	0.2	0.0	4.0	10.0

TIME DAY	HOUR	GRID NUMBER	TRAVEL TIME(HR)	CONSTI TUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			
							DECAY	DISP	LATC	TRIB
3	6.80	1	0.00	TEMP(C)	21.60	21.60	0.00	0.00	0.00	0.00
				ALGAE	0.00	0.00	0.00	0.00	0.00	0.00
				AMMONIA	0.01	0.01	0.00	0.00	0.00	0.00
				NITRITE	0.05	0.05	0.00	0.00	0.00	0.00
				NITRATE	0.24	0.24	0.00	0.00	0.00	0.00
				PHOSPHY	0.01	0.01	0.00	0.00	0.00	0.00
				BCD	4.10	4.10	0.00	0.00	0.00	0.00
				DISS O	9.20	9.20	0.00	0.00	0.00	0.00

CR(I1,I2)

I2	I1							
	1	2	3	4	5	6	7	8
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	8.698

XK(I1,I2)

I2	I1							
	1	2	3	4	5	6	7	8
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.000	-0.009	0.001	0.000	-0.000	0.000	0.000	-0.018
3	0.000	0.000	-0.013	0.013	0.000	0.000	0.000	-0.046
4	0.000	0.000	0.000	-0.117	0.117	0.000	0.000	-0.133
5	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7	0.000	0.000	0.000	0.000	0.000	0.000	-0.007	-0.007
8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.075

S(I1)

I1							
1	2	3	4	5	6	7	8
0.073	0.000	0.000	0.000	0.000	0.000	0.000	0.000

TIME DAY	HOOR	GRID NUMBER	TRAVEL TIME(HR)	CONSTITUENT	GRID CONC	PARCEL CONC AT ENTRY	CHANGE IN CONC DUE TO			
							DECAY	DISP	LATC	TRIB
7	5.55			TEMP(C)	22.2C	21.60	0.37	0.00	0.00	6.24
				ALGAE	0.00	0.00	0.00	0.00	0.00	0.00
				AMMONIA	1.72	0.01	-0.04	0.00	0.00	1.75
				NITRITE	0.06	0.05	0.01	-0.00	0.00	-0.00
				NITRATE	0.25	0.24	0.03	-0.00	0.00	-0.02
				PHOSPHY	0.38	0.01	0.00	0.00	0.00	0.37
				BOD	12.79	4.10	-0.27	0.00	0.00	8.96
				DISS O	8.47	9.20	-0.56	0.00	0.00	-0.17
8	7.27			TEMP(C)	28.38	21.60	0.21	0.00	0.00	6.56
				ALGAE	0.00	0.00	0.00	0.00	0.00	0.00
				AMMONIA	1.67	0.01	-0.10	0.00	0.00	1.76
				NITRITE	0.09	0.05	0.05	0.00	0.00	-0.01
				NITRATE	0.27	0.24	0.05	-0.00	0.00	-0.02
				PHOSPHY	0.38	0.01	0.00	0.00	0.00	0.37
				BOD	12.62	4.10	-0.49	0.00	0.00	9.02
				DISS O	7.99	9.20	-1.05	0.00	0.00	-0.16
25	43.56			TEMP(C)	25.18	21.60	-1.17	-0.00	0.00	4.75
				ALGAE	0.00	0.00	0.00	0.00	0.00	0.00
				AMMONIA	0.81	0.01	-0.86	0.00	0.00	1.65
				NITRITE	0.10	0.05	0.11	0.00	0.00	-0.05
				NITRATE	0.88	0.24	0.75	-0.00	0.00	-0.11
				PHOSPHY	0.37	0.01	0.00	0.00	0.00	0.36
				BOD	8.18	4.10	-3.87	0.00	0.00	7.95
				DISS O	4.25	9.20	-3.38	-0.00	0.00	0.43