

ENHANCEMENTS TO THE BRANCHED LAGRANGIAN TRANSPORT MODELING SYSTEM

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Enhancements to the Branched Lagrangian Transport Modeling System

By Harvey E. Jobson

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LIST OF SYMBOLS

| | |
|----------|--|
| a | coefficient in equation for total precipitable water content of the atmosphere |
| a' | atmospheric transmission coefficient to account for scattering |
| a'' | atmospheric transmission coefficient to account for absorption and scattering |
| A | cross-sectional area |
| AL | concentration of algae, mg/L |
| ALGSET | local settling rate for algae, ft/day |
| ALPH0 | conversion factor, mg Chlorophyll-A/mg Algae |
| ALPH1 | fraction of algal biomass that is nitrogen, mg-N/mg-Algae |
| ALPH2 | fraction of algae biomass that is phosphorus, mg-P/mg-Algae |
| ALPH3 | oxygen production per unit of algal growth, mg-O/mg-Algae |
| ALPH4 | oxygen uptake per unit of algae expired, mg-O/mg-Algae |
| ALPH5 | oxygen uptake per unit of NH_3 oxidation, mg-O/mg-N |
| ALPH6 | oxygen uptake per unit of NO_2 oxidation, mg-O/mg-N |
| b | coefficient in equation for total precipitable water content of the atmosphere |
| BET1 | rate constant for biological oxidation of NH_3 to NO_2 , per day |
| BET2 | rate constant for biological oxidation of NO_2 to NO_3 , per day |
| BET3 | rate constant for ON to NH_3 transformation, per day |
| BET4 | organic phosphorus decay rate, per day |
| CBOD | concentration of carbonaceous biological oxygen demand, mg/L |
| BR | branch for which the information applies |
| C | portion of sky covered by clouds |
| CB | exponent on flow for reaeration option 7 |
| CKL | light constant, $\text{cal/cm}^2/\text{min} = \text{Langley/min}$ |
| CKN | nitrogen half-saturation constant for algae, mg/L |
| CKP | phosphorus half-saturation constant for algae, mg/L |
| CK1 | carbonaceous CBOD decay rate, per day |
| CK2 | reaeration rate, per day |
| CK3 | carbonaceous CBOD sink rate, per day |
| CK4 | benthos consumption of oxygen, mg-O/day/ft^2 |
| C_p | specific heat of water at constant pressure |
| D_j | Julian day of the year |
| D_{ms} | maximum possible sunshine duration for the day |
| DO | concentration of dissolved oxygen, in mg/L |
| D_s | sunshine duration for the day |
| D_x | longitudinal dispersion coefficient |

| | |
|----------|--|
| e_a | vapor pressure of the air above the water |
| e_o | saturation vapor pressure of air evaluated at a temperature equal to that of the water surface |
| e_{op} | slope of the saturation vapor pressure curve with respect to temperature |
| E | rate of evaporation in units of length per time |
| ET | equation of time, assumed zero here |
| GR | subreach for which the information applies |
| GROMAX | maximum specific growth rate of algae, per day |
| HA | local hour angle |
| HA_r | complementary sunrise angle |
| H_b | heat flux caused by long-wave radiation emitted by the water |
| H_e | heat utilized by evaporation |
| H_h | heat conducted from the water as sensible heat |
| H_n | net heat flux caused by incoming radiation from the sun and the sky |
| H_{na} | net rate of heat absorption by the atmosphere |
| H_r | heat added by rain falling directly on the surface |
| H_s | rate of absorption of solar radiation by the atmosphere |
| H_t | net exchange of thermal energy between the air and the water |
| IGRO | growth rate option |
| K | kinetic surface exchange coefficient |
| K_a | heat exchange coefficient for the atmosphere |
| K2O | option for K_2 (reaeration coefficient input) |
| LFO | light function option |
| m_a | mass of air per unit area |
| m_o | optical air mass at sea level |
| m_p | local optical air mass |
| NH3 | concentration of ammonia, in mg/L as nitrogen |
| NO2 | concentration of nitrite, in mg/L as nitrogen |
| NO3 | concentration of nitrate, in mg/L as nitrogen |
| ON | concentration of organic nitrogen, in mg/L as nitrogen |
| OP | concentration of organic phosphorus, in mg/L as phosphorus |
| p | local barometric pressure |
| P | concentration of orthophosphate, in mg/L as phosphorus |
| PN | preference factor for ammonia nitrogen (0-1.0) |
| p_o | barometric pressure at sea level |
| r | radius vector of the sun |
| RSPRT | algal respiration rate, per day |

| | |
|----------|--|
| S_c | solar constant |
| S_{cc} | ground-level solar radiation intensity under a cloudy sky |
| S_e | extraterrestrial solar radiation intensity per unit area and time |
| SHAD0 | non-algal portion of light extinction coefficient, per ft |
| SHAD1 | linear algal self shading coefficient |
| SHAD2 | nonlinear algal self shading coefficient |
| SIG2 | benthos source rate for dissolved P, mg-P/ft ² /day |
| SIG3 | benthos source rate for NH ₃ , mg-N/ft ² day |
| SIG4 | organic nitrogen settling rate, per day |
| SIG5 | organic phosphorus settling rate, per day |
| S_o | solar radiation reaching the ground under a cloudless, dust-free, moist atmosphere |
| SONET | light intensity, cal/cm ² /min = Langley/min |
| ST | clock time, in hours |
| t | time |
| t_f | time of the first temperature extreme |
| t_s | time of the second temperature extreme |
| T | cross-sectional average water temperature |
| T_a | air temperature |
| TE | equilibrium temperature, degrees Celsius |
| T_h | the high air temperature for the day |
| TD | dewpoint temperature of the air, in degrees Fahrenheit |
| T_l | the low air temperature for the day |
| T_s | water surface temperature |
| U | stream velocity |
| V | wind speed, meter/second |
| w | total precipitable water content of the atmosphere |
| W | top width of the channel |
| x | longitudinal coordinate |
| z | the elevation of the point in question, in feet |

| | |
|-----------------|--|
| α | solar altitude |
| α_{sr} | altitude of the horizon at sunrise |
| δ | declination of the sun |
| ε | emissivity of water |
| ε_e | emissivity of air |
| π | constant 3.14159 |
| ρ | density of water |
| σ | Stefan-Boltzman constant for blackbody radiation |
| θ | phase angle |
| ϕ | latitude of the location |
| Ψ | an empirical coefficient or wind function dependent on wind speed |
| Ψ_l | longitude of the point in question, in degrees |
| Ψ_s | longitude of the time zone from which the clock time is measured, in degrees |

CONVERSION FACTORS AND ABBREVIATED WATER-QUALITY UNITS

| | Multiply | By | To obtain |
|--|----------|---------|--|
| inch (in.) | | 25.4 | millimeter (mm) |
| foot (ft) | | 0.3048 | meter (m) |
| foot/second (ft/s) | | 0.3048 | meter/second (m/s) |
| mile (mi) | | 1.609 | kilometer (km) |
| mile/hour (mph) | | 0.4470 | meter/second (m/s) |
| square foot (ft ²) | | 0.09290 | square meter (m ²) |
| square mile (mi ²) | | 2.590 | square kilometer (km ²) |
| cubic foot (ft ³) | | 0.02832 | cubic meter (m ³) |
| cubic foot per second (ft ³ /s) | | 0.02832 | cubic meter per second (m ³ /s) |
| kilopascal (kPa) | | 10.00 | millibar (mb) |
| inch of mercury at 60° F (in Hg) | | 33.7685 | millibar (mb) |
| milligram per day per foot (mg/day/ft) | | 3.2808 | milligram per day per meter (mg/day/m) |
| Langley | | 1.0000 | calorie per square centimeter (cal/cm ²) |
| British thermal unit (60°F) | | 252.04 | calorie (20°C) |

Temperature is given in degrees Celsius (°C), which can be converted to degrees Fahrenheit (°F) by use of the following equation:

$$^{\circ}\text{F} = 1.8(^{\circ}\text{C}) + 32$$

Temperature in degrees Celsius can be converted to degrees Kelvin (°K) by adding 273.16 or:

$$^{\circ}\text{K} = 273.16 + ^{\circ}\text{C}$$

Abbreviated water-quality units used in this report: Chemical concentrations and water temperature are given in metric units. Chemical concentration is given in milligram per liter (mg/L) or microgram per liter (µg/L). Milligram per liter is a unit expressing the concentration of chemical constituents in solution as weight (milligram) of solute per unit volume (liter) of water. One thousand microgram per liter is equivalent to one milligram per liter. For concentrations less than 7,000 mg/L, the numerical value is the same as for concentrations in parts per million.

ADDITIONAL ABBREVIATIONS

| | |
|-----------------|---------------------|
| °C | degree Celsius |
| cal | calorie |
| cm | centimeter |
| °F | degree Fahrenheit |
| ft ² | square foot |
| g | gram |
| hr | hour |
| °K | degree Kelvin |
| kPa | kilopascals |
| L | liter |
| m | meter |
| mb | millibar |
| mg/L | milligram per liter |
| mi | mile |
| mm | millimeter |
| min | minute |
| s | second |

ACRONYMS

| | |
|------------|--|
| BBLTM | Program to build input file "bltm.in" |
| BLTM | Branched Lagrangian Transport Model |
| BQUAL2E | Program to build input file "qual2e.in" |
| DAFLOW | Diffusion analogy flow model |
| EPA | U.S. Environmental Protection Agency |
| EPA-QUAL2E | Water-quality model developed by the EPA |
| EQU TMP | Program to estimate equilibrium temperatures |
| INTRP | Program to interpolate data to uniform spacing |
| MRG | Program to merge columns of data |
| NWS | National Weather Service |
| CTPLT | Program to plot concentration verses time at a specified river mile |
| CXPLT | Program to plot concentration verses river mile at a specified time |
| QUAL2E | Subroutine to BLTM code which mimics the reaction kinetics in the EPA code with the same name |
| SOLAR | Program to estimate solar radiation values |
| USGS | U.S. Geological Survey |
| TDDS | Time-Dependent Data System |

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Abstract

The Branched Lagrangian Transport Model (BLTM) has received wide use within the U.S. Geological Survey over the past 10 years. This report documents the enhancements and modifications that have been made to this modeling system since it was first introduced. The programs in the modeling system are arranged into five levels—programs to generate time-series of meteorological data (EQUULTMP, SOLAR), programs to process time-series data (INTRP, MRG), programs to build input files for transport model (BBLTM, BQUAL2E), the model with defined reaction kinetics (BLTM, QUAL2E), and post processor plotting programs (CTPLT, CXPLT). An example application is presented to illustrate how the modeling system can be used to simulate 10 water-quality constituents in the Chattahoochee River below Atlanta, Georgia.

INTRODUCTION

The Branched Lagrangian Transport Model (BLTM), as documented by Jobson and Schoellhamer (1987), has found wide use throughout the U.S. Geological Survey (USGS) and elsewhere (California Water Resources Control Board, 1996; Drewes and Conrads, 1995; Graf, 1995; Weiss and others, 1994; Bulak and others, 1993; Wiley, 1993). During the past several years, support programs have been written and some enhancements to the original code have been made. The purpose of this report is to document the support programs and enhancements to the BLTM model.

The BLTM model solves the one-dimensional advective dispersion equation by using a Lagrangian reference frame in which the computational nodes move with the flow. This solution scheme minimizes numerical dispersion and allows the user to tabulate the effect of each physical process on the computed concentrations. The BLTM model can route any number of interactive constituents for which the physical and (or) chemical reaction rates are defined in a subroutine; special subroutines have been developed to route, for example, rhotone, salinity, and bass eggs. Because the U.S. Environmental Protection Agency's (EPA) stream-water-quality model QUAL2 (EPA-QUAL2) was in wide use at the time the BLTM was published in 1987, the BLTM model was supplied with a subroutine called QUAL2 that simulated the reaction kinetics in the EPA model. The QUAL2 subroutine linked to BLTM allowed the EPA-QUAL2 kinetics to be applied to unsteady, reversing flow such as occurs in one-dimensional estuaries. This report documents a new subroutine, called QUAL2E, that simulates the reaction kinetics used in the newer version of the EPA-QUAL2E model (Brown and Barnwell, 1987).

The programs documented in this report can be divided into five levels of operation. Figure 1 is a schematic showing how they can be used to form a modeling system. The rectangular boxes represent programs and the ovals represent input or output data files.

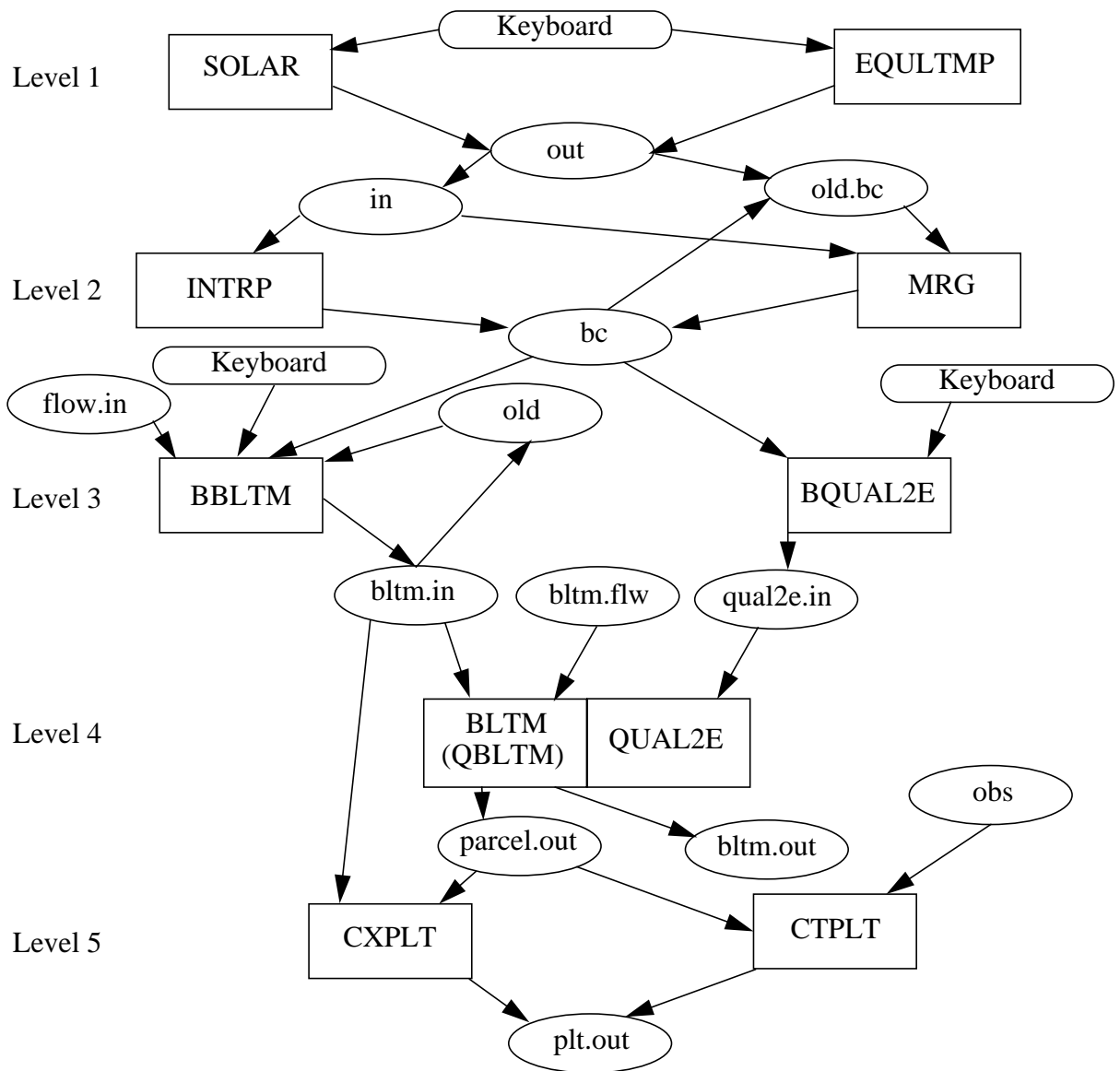
The first-level programs are designed to create the time series of meteorologic information needed by water quality models. Because most reaction rates depend on temperature, temperature will almost always be one of the constituents simulated. Any temperature model must be supplied with a time series of basic information, such as wind speed, equilibrium temperature, and, perhaps, solar radiation. The two programs shown at this level are designed to create these time series from information that is readily available from the National Weather Service (NWS).

The second-level programs are designed to process time-series data. The program INTRP is used to interpolate data from an uneven time series to produce a uniform time step. The program MRG is used to merge the second column of data from the file "in" to a specified column in a table of data contained in the file "old.bc".

The third-level programs are designed to query the user for input from the keyboard and to merge this information with time-series boundary conditions, which are read either from the keyboard or a file called "bc," and to write an input file for the model BLTM or its kinetics subroutine QUAL2E.

The BLTM model and the linked subroutine QUAL2E represent the fourth level in figure 1. The fifth-level programs, which are post processor programs, read output files to produce plots and/or compute basic statistics for the output. The CTPLT program plots concentration verses time for any specified river location and may compare the computed concentrations with observed values to compute the mean and root-mean-square error. The CXPLT program plots concentration verses distance at any specified time.

All USGS hydrologic analysis software is available for electronic retrieval by means of either the World-Wide Web at <http://water.usgs.gov/software/> and via anonymous File Transfer Protocol (FTP) from water.usgs.gov (path: /pub/software). The World-Wide Web page and the anonymous FTP directory from which the software discussed in this report can be retrieved are <http://water.usgs.gov/software/bltm.html> and [/pub/software/water_quality/bltm](http://water.usgs.gov/pub/software/water_quality/bltm), respectively.



The rectangles, SOLAR, EQULTMP, INTRP, MRG, BBLTM, BQUAL2E, BLTM, CXPLT, and CTPLT, represent programs in the Branched Lagrangian Transport Modeling system.

Data files, represented by ovals, include: in, out, bc, old.bc, flow.in, old, bltm.in, bltm.flw, qual2e.in, parcel.out, bltm.out, obs, and plt.out. These are used either as input or output to the programs. Information moves in the direction of the arrows.

Figure 1. Schematic of programs and file structure used in Branched Lagrangian Transport Modeling system.

LEVEL 1—PROGRAMS TO GENERATE METEOROLOGICAL TIME SERIES (EQUULTMP, SOLAR)

Program to Estimate Equilibrium Temperatures From Air Temperature (EQUULTMP)

The program EQUULTMP estimates equilibrium water temperature from wind speed and the daily maximum and minimum air temperatures. These variables are recorded by the NWS at many sites throughout the country.

Theory

The problem of temperature prediction in rivers is dependent on predicting the equilibrium temperature. Although the rate of exchange of energy between the water and the atmosphere has been discussed many times, Anderson (1954) provided one of the first and most complete analyses of the processes involved. Following Anderson's lead, the net exchange is expressed as the sum:

$$H_t = H_n + H_r - H_b - H_e - H_h, \quad (1)$$

where H_t = the net exchange of thermal energy between the air and the water; H_n = net heat flux caused by incoming radiation from the sun and the sky; H_r = heat added by rain falling directly on the surface; H_b = heat flux caused by long-wave radiation emitted by the water; H_e = heat utilized by evaporation; and H_h = heat conducted from the water as sensible heat. If the water is gaining thermal energy as a result of the respective processes, the values of H_t , H_n , and H_r are positive and those of H_b , H_e , and H_h are negative.

All objects at temperatures above absolute zero emit radiant energy. The amount of radiant energy emitted by an object can be computed by use of Stefan's law which is mainly a function of the surface temperature.

The emitted energy is distributed over a wavelength range, and Wien's law can be used to determine the wavelength which has the maximum intensity. At the sun's temperature (about 6,000 degrees Kelvin [$^{\circ}\text{K}$]) the wavelength of the emitted radiation peaks at about 0.5 micrometer and ranges from about 0.3 to 2.2 micrometer. This range roughly corresponds to the visible spectrum. The temperature of the molecules in the atmosphere, however, is about 300 $^{\circ}\text{K}$; so the atmosphere emits radiation in the wavelength range of 7 to 100 micrometer, which cannot be detected by the human eye. Because different types of instruments are used to detect these two types of radiation; they are generally considered separately in the energy balance.

Figure 2 shows the daily averaged value of the surface-exchange terms for the San Diego Aqueduct for a winter and a summer day to illustrate the relative magnitudes. The San Diego Aqueduct is located in Southern California, which has a hot, dry climate where the evaporation term is large. All terms except solar radiation generally vary mildly throughout the day, perhaps 25 percent. The solar radiation term varies from zero at night to a maximum at solar noon on a clear day and also can vary greatly during a partly cloudy day.

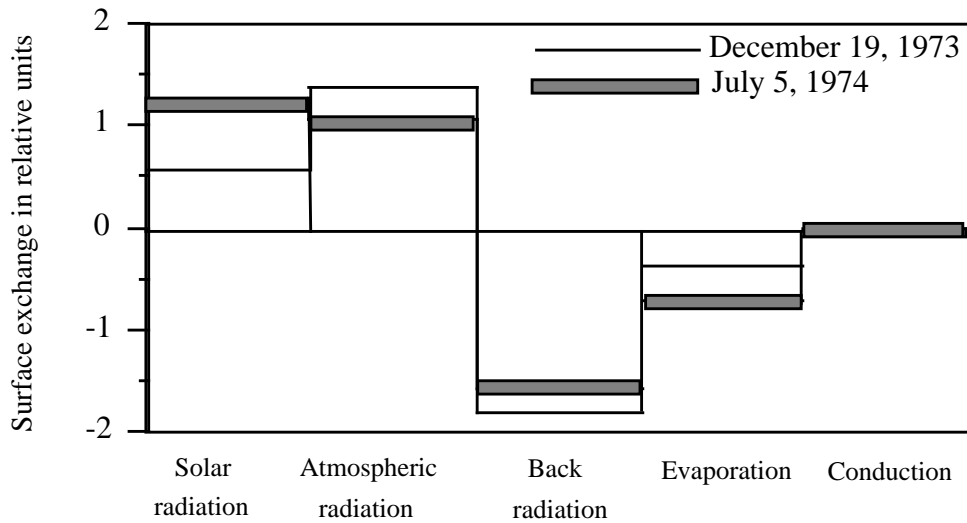


Figure 2. Relative values of daily average surface-exchange terms resulting from various processes for typical days on the San Diego Aqueduct.

The flux caused by incoming radiation from the sun and the sky, H_n , is usually broken into four components—the incoming atmospheric and solar radiation and the reflected parts of each. The incoming components are often measured directly, but the reflected parts are usually estimated from various formulas. Usually 3 percent of the atmospheric radiation is assumed to be reflected. The reflected part of the solar radiation varies with the altitude of the sun but averages about 6 percent for the day. Various formulas for computing the incoming solar and atmospheric radiation are summarized by Wunderlich (1972, p. 4.20). The two components can be of equal size on a daily average basis. The atmospheric component can be computed fairly accurately, but the solar component can be very difficult to compute on a cloudy day.

All the other terms in equation 1 are a function of the water temperature; so they must be computed by using analytic expressions. Expressions that can be used are given below.

Long-wave radiation emitted by the water surface is usually computed by using the Stefan-Boltzman law:

$$H_b = \varepsilon \cdot \sigma \cdot (T_s + 273.16)^4, \quad (2)$$

where ε = emissivity of water (0.97); σ = Stefan-Boltzman constant for blackbody radiation (1.171×10^{-7} calorie/day/cm²/°K⁴); and 273.16 converts to the Kelvin scale when T_s , the water surface temperature, is given in degrees Celsius. It is normal practice to assume the water surface temperature is equal to the cross sectional average water temperature, T .

The rate of evaporation is usually estimated by a formula of the Dalton type:

$$E = \psi \cdot (e_o - e_a), \quad (3)$$

where E = rate of evaporation in units of length per time; ψ = an empirical coefficient or wind function dependent on wind speed; e_o = saturation vapor pressure of air evaluated at a temperature equal to that of the water surface; and e_a = vapor pressure of the air above the water, which is commonly measured at a height equal to the height of the measured wind speed. The saturation vapor pressure of air at a temperature T can be approximated as:

$$e_o = \exp\left(52.4185 - \frac{6788.6}{T + 273.16} - 5.0016 \cdot \ln(T + 273.16)\right), \quad (4)$$

where e_o is given in kilopascals (kPa) and T is given in degrees Celsius. Equation 4 provides estimates of published vapor pressures (Hodgman, 1960) in the range of 0 to 40 degrees Celsius ($^{\circ}\text{C}$) with a root-mean-square error (RMS) of 0.0004 kPa, a maximum percentage error of -0.037 percent at 4 $^{\circ}\text{C}$, and a maximum absolute error of -0.022 kPa at 40 $^{\circ}\text{C}$.

Empirical wind functions derived from lake or pan data are numerous (Ryan and Stolzenbach, 1972; Wunderlich, 1972; Brutsaert and Yeh, 1970) but they usually take the form:

$$\psi = 0.301 + 0.113 \cdot V, \quad (5)$$

where ψ = wind function that gives the evaporation, in centimeter per day when the vapor pressure deficit is expressed in kilopascals; and V = wind-speed, expressed in meter per second. The constants 0.301 and 0.113 were derived from a thermal balance of the San Diego Aqueduct (Jobson, 1977). The second constant (0.113) is often called the mass transfer coefficient for evaporation.

The thermal energy utilized by evaporation is expressed as:

$$H_e = \rho \cdot L \cdot \psi \cdot (e_o - e_a), \quad (6)$$

where ρ = density of water, in g/cm^3 ; and L = latent heat of vaporization of water (595 - 0.045 T , in cal/g).

The heat exchanged by conduction is generally smaller than the evaporative heat exchange. Assuming that the eddy diffusivity of heat and mass are identical, which leads directly to the Bowen ratio concept, the conduction term can be expressed as:

$$H_h = \gamma \cdot \rho \cdot L \cdot \psi \cdot (T - T_a), \quad (7)$$

where γ = psychrometric constant, in $\text{kPa}/^{\circ}\text{C}$ (0.598 based on an assumed atmospheric pressure of 98.0 kPa); and T_a = air temperature, in degrees Celsius, which should be measured at the same elevation as the vapor pressure.

The energy added by rainfall is determined by:

$$H_r = C_p \cdot \rho \cdot I \cdot (T_w - T), \quad (8)$$

where C_p = specific heat of water at atmospheric pressure, in cal/g/°C; I = rainfall rate, in cm/day; and T_w = wet-bulb air temperature, in degrees Celsius.

When equations 3 through 8 are combined with equation 1, the surface heat exchange is seen to be a function of water temperature, as shown on figure 3. For the conditions assumed in figure 3 the net surface exchange becomes zero at a temperature of about 16 °C, because the heat gained from the sun and the sky is just balanced by the heat lost to back radiation, evaporation, and conduction. The temperature at which the net surface exchange becomes zero is defined as the "equilibrium temperature". A stagnant pool of water would approach this temperature and remain constant if the external conditions (solar radiation, atmospheric radiation, wind speed, air temperature, and relative humidity) remained constant. It is often easier to estimate the equilibrium temperature directly than to measure or estimate all the meteorologic parameters needed to compute it.

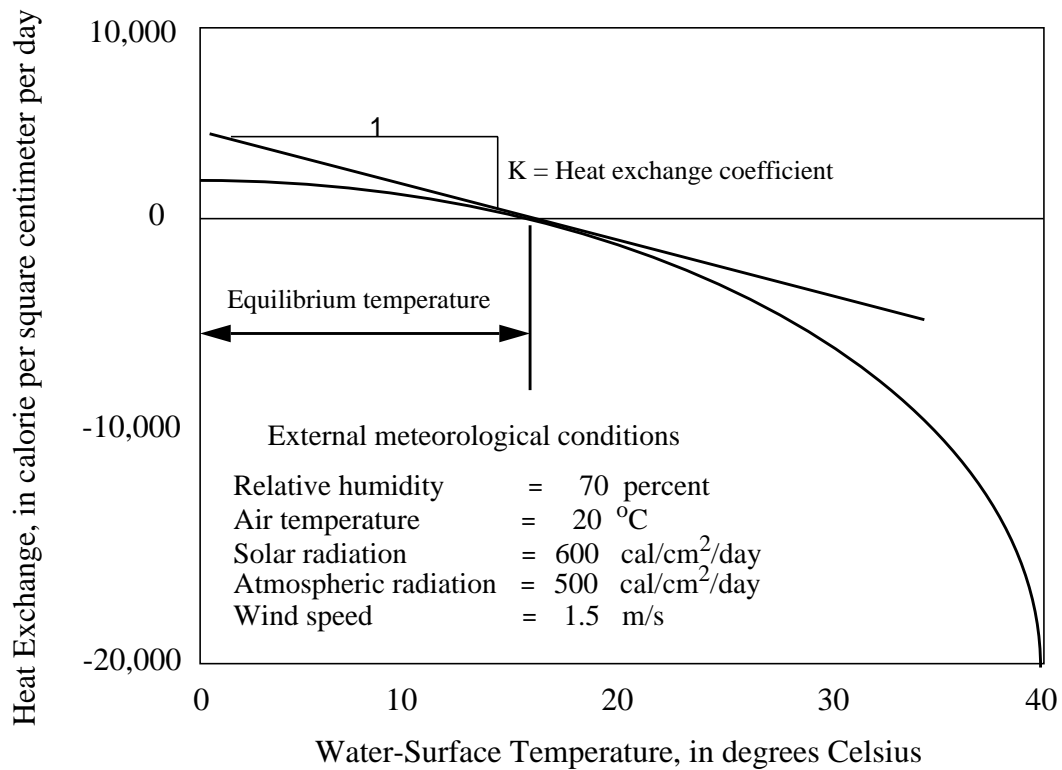


Figure 3. Total surface exchange as a function of water-surface temperature.

The ultimate heat source for the atmosphere, as well as any water body, is the incoming solar radiation, some of which is absorbed by the air and some of which is transmitted to the Earth's surface. The dominant heat sink for the atmosphere is back radiation so the rate of heat absorption by the atmosphere can be approximated as:

$$H_{na} = H_s - \epsilon_e \cdot \sigma \cdot T_a^4, \quad (9)$$

where H_{na} = net rate of heat absorption by the atmosphere, H_s = rate of absorption of solar radiation by the atmosphere, and ϵ_e = emissivity of air. As can be seen from the form of equation 9, an equilibrium temperature (T_e) also can be defined for the atmosphere because for any given rate of incoming solar radiation, there will be one air temperature for which the net heat exchange will be zero. If the incoming solar radiation, H_s , were to suddenly change, then the equilibrium air temperature also would suddenly change, but the air temperature would only gradually approach the new equilibrium value. The rate at which the air approached the new equilibrium temperature could be computed from:

$$\frac{\partial T_a}{\partial t} = \frac{K_a \cdot (T_a - T_e)}{m_a}, \quad (10)$$

where m_a = mass of air per unit area, and K_a = heat exchange coefficient for the atmosphere as computed from:

$$K_a = \frac{\partial H_s}{\partial T_a} = 4 \cdot \epsilon_e \cdot \sigma \cdot T_a^3. \quad (11)$$

For a stagnant atmosphere (no cold or warm fronts moving into a region) the variation of air temperature at a point should be closely approximated by using equations 9 through 11. So assuming the values of K_a and m_a are constant, the time variation of equilibrium temperature for the atmosphere can be computed from an observed variation in air temperature by using these equations.

When averaged over a long period of time (a week to a month) the water temperature of a river or lake is normally observed to be nearly equal to the average air temperature for the same period. This seems to be a reasonable observation if both are responding to the same forcing function, which is dominated by solar radiation. If both approach the same temperature when averaged over time, then it also seems reasonable to assume that the same equilibrium temperature applies to the air and the water. Thus, the equilibrium temperature, as computed from the time variation of air temperature, can be assumed to be applicable to a water body. The approximation should be most valid for a stagnant air mass and least accurate when the variation of air temperature with time is dominated by the advection of a cold or warm front through the area. At any instant, the temperatures of air and water are different mainly because of the differing thermal masses.

The program EQUQTMP assumes that the equilibrium temperature of the air and water are equal and that the air temperature varies as a sine function between the daily extremes. With these assumptions, the time variation of equilibrium temperature can be computed as:

$$T_e = T_a + \frac{K_a \cdot (T_h - T_l)}{2 \cdot m_a \cdot (t_s - t_f)} \cdot \cos(t + \theta), \quad (12)$$

where T_h = high temperature extreme, T_l = low temperature extreme, t_f = time of first temperature extreme, t_s = time of second temperature extreme, t = time, and θ = the phase angle ($3\pi/2$ if the first extreme is the minimum temperature, and $\pi/2$ if the first extreme is the maximum temperature). The value of K_a/m_a (the thermal mass of the atmosphere) can be determined from the mean lag between the time of the peak equilibrium temperature (solar noon) and the time of the peak air temperature. The default value given in the model assumes that the peak air temperature occurs at 4 hours past solar noon.

The program EQUULTMP computes the equilibrium temperature from equation 12. This assumption greatly simplifies the task of computing an equilibrium temperature and eliminates the need for extensive data that are difficult to obtain.

Input, Output, and Operation

The keyboard is used to supply all input for the program EQUULTMP. First, the program requests the user to supply the time step to be used in the transport model and the text information to be written as the first line of the output file. It then requests the input for the thermal mass of the atmosphere.

Next, the maximum temperature and its time of occurrence are requested for the day that precedes the day when the equilibrium temperatures are desired. Then, the minimum temperature, the time of occurrence, and the average wind speed for the day are requested. With this information, the program computes the equilibrium temperatures between midnight and the time of the morning minimum (from eq 12). The first equilibrium temperature is computed as that which occurs at one-half time step past midnight (the center of the time step). With the equilibrium temperatures computed and printed to the output file for times from midnight to the time when the air temperature is at the minimum, the program requests the daily maximum temperature and the time of occurrence to compute the equilibrium temperatures for the middle part of the day. With the equilibrium temperatures computed up to the time of the maximum air temperature for the day, the program requests the minimum temperature and the time of occurrence, for the day following the day being computed and completes the computations for the day. The program finally asks if another day is to be computed and either terminates or repeats the cycle.

The results are written to a file called "out," which can be merged with solar radiation data and used as input for QUAL2E. The output consists of two lines of text information and four columns of data. The first line of text in the output is input by the user for information purposes, and the second line of output consists of column headings generated by the program. These two lines are ignored in all later analyses. The data columns include the time, in hours; the equilibrium temperature, in degrees Celsius; the wind speed, in meter per second; and the air temperature, in degrees Celsius. The air temperature is not used by QUAL2E, but is output by EQUULTMP for information purposes.

Program to Estimate Incoming Solar Radiation (SOLAR)

The subroutine QUAL2E simulates the growth of algae, which is dependent on the amount of available solar radiation that are input as boundary conditions. Ideally, measured values are available to be used as input, but more commonly the values are not available. The program SOLAR is designed to estimate incoming solar radiation levels that are based on information generally available from the NWS.

Theory

The theory upon which the program is based has been presented by Wunderlich (1972) and is summarized below for convenience. The computations proceed along three steps—compute the solar radiation received at the top of the atmosphere above the point in question, adjust to ground level values by accounting for attenuation as it passes through a clear sky, and, finally, reduce the amount further to account for cloud cover.

The computation of solar radiation received at the top of the Earth's atmosphere is based on known values of radiation emitted by the sun and the trigonometric relation between the direct solar beam and its component on a plane tangent to the surface of the atmosphere directly above the point in question. The solar radiation intensity on a horizontal plane at the top of the atmosphere is given (Wunderlich, 1972, p. 2.2) as:

$$S_e = \frac{S_c}{r^2} \cdot \sin \alpha, \quad (13)$$

where S_e = extra-terrestrial solar radiation intensity per unit area and time, S_c = solar constant, r = radius vector, and α = solar altitude determined by:

$$\sin \alpha = \sin \phi \cdot \sin \delta + \cos \phi \cdot \cos \delta \cdot \cos HA, \quad (14)$$

where ϕ = latitude of the location, δ = declination of the sun, and HA = local hour angle of the sun. Wunderlich (1972, p. 2.4) concluded that the radius vector and the declination of the sun can be assumed to be constant for any day and can be estimated from:

$$r = 1 + 0.017 \cdot \cos\left(\frac{2\pi}{365} \cdot (186 - D_j)\right), \quad (15)$$

and

$$\delta = 23.45 \cdot \frac{\pi}{180} \cdot \cos\left(\frac{2\pi}{365} \cdot (172 - D_j)\right), \quad (16)$$

where D_j = Julian day of the year.

The local hour angle is the angle measured westward around the axis of the celestial sphere (Earth) from the meridian of the observation point to the meridian of the sun; or expressed in a different way, the local hour angle is the angle that the Earth has turned since the sun was at the highest point in the sky relative to a local observer. The local hour angle, in hours, can be determined from clock time by using the expression:

$$HA = ST \pm 12 + \frac{(\psi_s - \psi_1)}{15} + ET, \quad (17)$$

where ST = clock time, in hours; ψ_s = longitude of the time zone (degrees) from which ST is measured; ψ_1 = longitude of the point in question (degrees); and ET = the equation of time. The 15 in equation 17 should be changed to -15 for points of east longitude and the sign of the 12 is selected such that the absolute value of HA remains less than 24 hours. The equation of time accounts for apparent movement of the sun relative to the simple daily and annual cycles. The value of ET can be determined for any day from a solar ephemeris; its absolute value will always be less than 16 minutes. The equation of time, ET , is assumed to be zero in the SOLAR program. The value of HA is converted to degrees or radians in the usual manner for use in trigonometric expressions.

Equation 13 can be integrated over any time period (Wunderlich, 1972, p 2.8) to give:

$$S_e = \frac{S_c}{(t_2 - t_1) \cdot r^2} \cdot \left((t_2 - t_1) \cdot \sin \phi \cdot \sin \delta + \frac{12}{\pi} \cdot \cos \phi \cdot \cos \delta \cdot (\sin HA_2 - \sin HA_1) \right), \quad (18)$$

where S_e = average solar radiation received on a horizontal plane at the top of the atmosphere between time t_1 and t_2 ; t_1 = time at start of period; t_2 = time at end of period; HA_1 = local hour angle at beginning of the period; and HA_2 = local hour angle at end of the period.

The time of sunrise or sunset is defined as the time when the center of the sun is at the altitude of the horizon. For an observer on a flat plane, the altitude of the horizon would be zero, for an observer to the west of a large hill or mountain, however, the altitude of the sunrise would be greater than zero. The hour angle of sunrise is computed from (Wunderlich, 1972, p 2.9) as:

$$\cos HA_r = \frac{\sin \alpha_{sr} - (\sin \phi \cdot \sin \delta)}{\cos \phi \cdot \cos \delta}, \quad (19)$$

where HA_r = complementary sunrise angle, and α_{sr} = the altitude of the horizon at sunrise. The local hour angle at sunset is computed from the same equation with the angle of the horizon at sunset replacing α_{sr} . The clock time of sunrise or sunset is determined from the local hour angle using equation 17. The first non-zero time period of the day integrates equation 18 from sunrise until the end of the time step and the last non-zero period of the day integrates from the start of the time step until sunset, not the end of the time period.

The solar radiation available at the top of the atmosphere, S_e , is reduced to account for attenuation as it passes through the atmosphere. Scattering and absorption by gases, water vapor, and dust cause the attenuation. Wunderlich (1972, p 2.12) used the approach of Klein (1948) to account for scattering and absorption in a dust-free atmosphere. The expression used is:

$$S_o = S_e \cdot (a'' + 0.5 - 0.5 \cdot a') , \quad (20)$$

where S_o = the solar radiation reaching the ground under a cloudless, dust-free, moist atmosphere; a'' = atmospheric transmission coefficient to account for absorption and scattering; and a' = atmospheric transmission coefficient to account for scattering. The effect of dust on the absorption is ignored in the SOLAR program. Both a'' and a' are functions of the optical air mass and the moisture content of the atmosphere.

The optical air mass is approximated using an equation established by Kasten (1964):

$$m_o = \frac{1}{\sin \alpha + 0.15 \cdot (\alpha + 3.885)^{-1.253}} , \quad (21)$$

where m_o = optical air mass at sea level, and α = solar altitude, in degrees. At elevations other than sea level, the air mass has to be adjusted according to the local barometric pressure by:

$$m_p = \frac{p}{p_o} \cdot m_o , \quad (22)$$

where m_p = local optical air mass, p = local barometric pressure, and p_o = barometric pressure at sea level. The SOLAR model assumes that the barometric pressure at sea level is 29.93 inches of mercury (101.35 kPa). The program also gives the user the option of specifying the station elevation rather than the local barometric pressure. When elevation is specified, the program computes the local optical air mass from the expression:

$$m_p = m_o \cdot \left(\frac{288 - (0.00198 \cdot z)}{288} \right)^{5.256} , \quad (23)$$

where z = the elevation of the point in question, in feet.

The total precipitable water content of the atmosphere is estimated from the dewpoint by using (Reitan, 1963):

$$w = e^{a + b \cdot TD} , \quad (24)$$

where w = total precipitable water content of the atmosphere, TD = the dewpoint temperature of the air, in degrees Fahrenheit, and the coefficients a and b are obtained from the following table.

Coefficients for use in equation 24 (from Reitan, 1963, p. 777):

| Station | a | b |
|-----------------------|--------|--------|
| Columbia, Mo. | -0.846 | 0.0325 |
| Grand Junction, Colo. | -1.304 | 0.0476 |
| Great Falls, Mont. | -1.092 | 0.0396 |
| Greensboro, N.C. | -0.975 | 0.0345 |
| Lake Charles, La. | -0.930 | 0.0328 |
| Medford, Oreg. | -1.292 | 0.0425 |
| Midland, Tex. | -1.022 | 0.0354 |
| Oklahoma City, Okla. | -0.956 | 0.0343 |
| Phoenix, Ariz. | -1.453 | 0.0436 |
| Portland, Maine | -0.925 | 0.0336 |
| St. Cloud, Minn. | -0.878 | 0.0321 |
| Santa Maria, Calif. | -1.192 | 0.0373 |
| Tampa, Fla. | -1.378 | 0.0396 |
| Tatoosh Island, Wash. | -1.466 | 0.0429 |
| Washington, D.C. | -0.948 | 0.0345 |
| Mean of 15 stations | -0.981 | 0.0341 |

The values of a'' and a' for use in equation 20 are estimated from the relations given by Water Resources Engineers, Inc. (1968, p. 41):

$$a' = e^{-(0.465 + 0.134 \cdot w) \cdot (0.129 + 0.171 \cdot e^{-(0.880 \cdot m_p)}) \cdot m_p}, \quad (25)$$

$$a'' = e^{-(0.465 + 0.134 \cdot w) \cdot (0.179 + 0.421 \cdot e^{-(0.721 \cdot m_p)}) \cdot m_p}. \quad (26)$$

Two methods for reducing the incoming radiation to account for cloud cover are allowed in the program. One method uses the ratio of sunshine duration to the maximum possible sunshine duration, as determined by the time between sunrise and sunset. The ground-level solar radiation intensity under a cloudy sky, S_{cc} , is estimated from an equation (Wunderlich, 1972, p. 2.19):

$$S_{cc} = \left(0.22 + 0.78 \cdot \left(\frac{D_s}{D_{ms}} \right)^{0.6667} \right) \cdot S_o, \quad (27)$$

where D_s = sunshine duration for the day, and D_{ms} = maximum possible sunshine duration for the day.

The second method of accounting for cloud cover is based on an estimate of the percentage of the sky covered by clouds (Wunderlich, 1972, p. 2.19):

$$S_{cc} = \left(1 - 0.71 \cdot C^2 \right) \cdot S_o, \quad (28)$$

where C = portion of sky covered by clouds which ranges from 0 to 1.0. The cloud cover and sunshine duration for many locations throughout the country are published by the NWS.

Input

Generally, the information published by the NWS will provide sufficient input to the program. The required input information includes the following:

- Time step size, in hours;
- User defined title information for output file;
- Solar constant, default = $1.95 \text{ cal/cm}^2/\text{min}$;
- Julian day of the start of the model;
- Longitude of the site, in degrees;
- Longitude of the local time meridian, in degrees;
- Latitude of the site, in degrees;
- Altitude of the sunrise horizon, in degrees;
- Altitude of the sunset horizon, in degrees;
- Either elevation of site, in feet, or
atmospheric pressure, in inches of mercury;
- Coefficients in empirical equation to determine precipitable water content of the atmosphere,
default values provided;
- Either cloud cover or
sunshine duration, in hours; and
- Dewpoint temperature, in degrees Fahrenheit.

Output and Operation

The program is designed to receive all input from the keyboard and to output a file called "out." The total solar radiation received during each time step of the day is computed. The output file begins with two lines of text information; the first line is for identification purposes only and is simply the title input by the user and the second line consists of program-generated column headings— "Time," "Lang," "Clear," and "Extra." Time is the time at the midpoint of the time step that starts at one-half time step past midnight and ends one-half time step before midnight for the day. The headings "Lang," "Clear," and "Extra" indicate the ground-level solar radiation intensity under a cloudy sky, S_{cc} ; the solar radiation that would reach the ground under a cloudless, dust-free, moist atmosphere, S_o ; and extraterrestrial solar radiation, S_e , respectively. The units in the output are the same as those used to input the solar constant. After the program has computed the radiation for each time step of the day, it queries the user to see if it should quit or increase the Julian day by one and compute radiation values for the next day.

LEVEL 2—PROGRAMS TO PROCESS TIME-SERIES DATA (INTRP, MRG)

Once time series of information are available, these values often need to be processed before they can be used directly as input to the transport program. For example, the spacing of the time steps may need to be modified or a table of values with multiple columns may need to be generated. If other software is not available to perform these functions, then the programs INTRP and MRG can be used. In general, files of time-series data are read as space-delimited free format, which means that the data can be in any format as long as the numbers are separated by at least one blank space. The first column is generally considered to be time, but it is not used by any programs except INTRP and CTPLT.

Program to Interpolate Data to Uniform Spacing (INTRP)

The program INTRP is designed to read data from a file called "in," which contains the abscissa (time) in the first column and an ordinate (flow, concentration, and so forth) in the second column, and to interpolate the ordinates (by using straight line interpolation between points occurring before and after the abscissa desired) to a uniform spacing along the abscissa. The results are written to a file called "bc."

The first two lines of the file "in" are simply read into the program as characters and written to the file "bc." These two lines can be used to identify the data in the file. Following the first two lines, the input file must contain at least two columns of numbers separated by at least one blank space; the format of the numbers is immaterial. The first column—the abscissa (usually time)—must have values that increase sequentially with the first value being less than or equal to the first abscissa to be interpolated, and the last value being equal to or larger than the last abscissa to be interpolated. The second column contains the ordinate values to be interpolated. The program ignores any other columns of data.

The program states that it will read a file called "in" and write a file called "bc." If these files are not available or if the file "bc" contains information that should not be lost, then the operator can abort the program at this point. The program then reads the file "in" and queries the operator for the "starting value of x," which is the abscissa value for which the first ordinate will be interpolated and written in the file "bc." The program next queries the operator for the "value of DX," which is the abscissa interval between the interpolated points. Finally, the program queries the operator for the "number of points to be interpolated" and the desired format of the output. Two output formats are available—the flow option writes the output in the format 2G12.4, and the transport option writes the output in the format 2F7.2.

Program to Merge Columns of Data (MRG)

Input files often require tabular input with multiple columns. For example, the initial or boundary conditions for a model with multiple constituents require input tables in which each column represents a time series of values for a specific constituent. Frequently the values in a specific column of a file need to be modified while leaving the rest of the table of data unchanged. Many text editors allow this operation to be performed with ease; if these editors are not available, however, the task can be very difficult to perform. The program MRG has been designed to facilitate this operation if a versatile text editor is not available. The output of the programs EQUPTMP and SOLAR also can be merged into a single file by using this program.

The program MRG reads two files, "old.bc" and "in," and writes one file, "bc." The file "bc" will be identical to the file "old.bc" except that a designated column (not counting the time column) will have been replaced by the second column of the file "in."

All files will contain two lines of text at the beginning followed by a table of numbers. The two lines of text in the file "old.bc" will be read and written to "bc." The first two lines of the file "in" will be ignored, and the second column of numbers will be read. All columns of the file "old.bc" will be read, and the program replaces one of these columns with that obtained from the file "in." The results are written to the file "bc." The data format in files "in" and "old.bc" is immaterial as long as each column of data is separated by at least one space.

The program first lists the files that will be read and written. If these files are not available or the output file contains information the user does not want to lose, then the program can be aborted at this time. If the program is not aborted, it queries the user for the output "format type desired" and the "number of data columns in *old.bc*". Two output formats are allowed—F7.2 or G12.4. If more than 20 columns are to be read, then the program must be re-dimensioned. The program queries the user for "column no. (excluding time) to be changed." The columns in the file "old.bc" are numbered from left to right starting with the second column.

LEVEL 3 —PROGRAMS TO BUILD INPUT FILES (BBLTM, BQUAL2E)

Program to Build Input File "bltm.in" (BBLTM)

The BLTM requires a rather large and complex input file called "bltm.in." Much of the required information for this file, such as the grid locations, branch numbers, and so forth, will generally be available in the file needed to run the flow model. The program BBLTM is designed to create the file "bltm.in" by combining information input from the keyboard with that in either the file "flow.in" (used to operate the DAFLOW model, (Jobson,1989)), or "old," and/or the file "bc" (see fig. 1). The program can be used either to create a new "bltm.in" file, in which case the file "flow.in" is read, or to edit an existing file, in which case the file "old" is read.

The data in "bltm.in" can be broken into two groups—the header, geometry, and initial conditions form one group and the boundary conditions form the other group. Only the boundary conditions can be edited with BBLTM. The other information can be easily modified using any full-screen editor. The information and format of the data in "bltm.in" are defined in detail in Jobson and Schoellhamer (1987, Appendix A).

The following sequence of operations is used to create a new file. The program reads title information from the file "flow.in," prints it to the screen, and requests new title information for "bltm.in." The title information is then printed, and the program requests the number of time steps between printouts in file "parcel.out" and the number of constituents to be modeled. It reads the numbers of branches, interior junctions, time steps to be modeled, time steps between midnight and the start of the model, time steps between printouts to "bltm.out", and type of units to be used from the file "flow.in." It then writes the fixed-point header card (Jobson and Schoellhamer, 1987, Appendix A) and assumes that the hydraulic information in the file "bltm.flw" is of the form produced by the flow model DAFLOW (ITDDS=0). Next, it reads the time-step size from "flow.in," requests the minimum dispersive velocity, and writes the floating-point header card. The titles for the constituents to be modeled and the constituent number (LR) for which reactions will be tabulated by the variable PDC are requested and printed as the constituent-labels data set. For each branch and subreach, the program then reads the available information from "flow.in" and request the initial number of parcels per subreach, the dispersion factor, the initial concentrations and output grids for each subreach. To determine the grids for which output is desired in "bltm.out," the program displays:

```
For branch          1
Enter an output GRID (enter q to quit).
```

If no output is desired for the indicated branch, then enter the letter "q" to quit; otherwise, enter the grid numbers, one at a time, where output is desired and enter "q" after all the desired grids have been entered. The program then writes all branch information to complete the first part of the input data.

The program next asks if the user wishes to enter a boundary condition from the file "bc." Only one boundary condition can be entered from this file. If the user responds in the affirmative, the program asks which branch and grid the boundary condition applies to. It then asks if the operator would like to enter any boundary conditions from the terminal.

If boundary conditions are input from the terminal, then for each time step, the program asks how many boundary conditions are to be input. For each boundary condition, it asks for the branch and grid number of the desired input, as well as the boundary value. Any number of boundary conditions can be input this way, and the number does not have to be the same for each time step. The BLTM assumes boundary conditions remain constant unless changed by the input.

The program BBLTM also can be used to change one or more boundary conditions after "bltm.in" is created. This is done by copying the file "bltm.in" to the file "old" and selecting the option to edit an existing file. When this option is selected, the BBLTM simply copies all information except the boundary conditions from the file "old" to the file "bltm.in" and then asks the user if boundary conditions are to be read from the file "bc" or the terminal. For each time step, all boundary conditions are first read from the file "old," then from the file "bc" (if this option is selected), and finally from the terminal (if this option is selected). If new boundary conditions are read in, they replace those already in memory so the boundary conditions in the file "bc" will replace those in "old" if both files have values for the same branch and grid. Likewise, the values entered from the keyboard (if this option is selected) will replace the values obtained from either "old" or "bc." Finally, all boundary conditions are written to the file "bltm.in."

If multiple boundary conditions are to be entered by using the file "bc," then the program BBLTM must be run once for each boundary condition. The file "bltm.in" is copied to the file "old" after each boundary condition is input.

Program to Build Input File "qual2e.in" (BQUAL2E)

When the subroutine QUAL2E is linked to the BLTM, the resulting transport model is often called QBLTM. QBLTM then simulates the reaction kinetics in the EPA-QUAL2E model. These reaction kinetics are defined by a large number of coefficients, many of which are variable from reach to reach. Likewise, the subroutine requires values of equilibrium temperature, wind speed, and solar radiation. The coefficients and input conditions are read from the large, complex file "qual2e.in." The program BQUAL2E is designed to help the user create this file. This program has no capability to edit coefficients in an existing input file, but the structure of the file is designed so that coefficients can be easily identified and edited by using a full screen editor.

After requesting and writing one line of title information, BQUAL2E lists each coefficient needed by the model, displays the assumed default value, and requests a new value. The desired coefficient can be entered from the keyboard, or the default can be selected by entering any letter.

Once the coefficients that are constant throughout the model have been entered and written to "qual2e.in," the number of branches is input. For each subreach of each branch, the user inputs the reach/variable coefficients. If a value is entered it becomes the default.

Then the number of time steps to be modeled is entered. All meteorologic data (equilibrium temperature, wind speed, and incoming solar radiation) are assumed to be constant for all branches and subreaches but are variable with time. Therefore, a different value is required for each time step. These values can be input from the keyboard or read from file "bc." If the data are read from the file "bc," the program simply reads these values for each time step and writes them to the file "qual2e.in." If the values are to be entered from the terminal, then the program requests the values and writes them to the file. The last number entered becomes the default.

LEVEL 4—BRANCHED LAGRANGIAN TRANSPORT MODEL (BLTM)

Enhancements to BLTM

Other than for minor coding changes to correct annoying bugs or to simplify the code, the BLTM has not been updated except for the five following modifications.

Reach Variable Dispersion Factor

The original code assumed the dispersion coefficient would remain constant within any branch. It was soon found that this coefficient needed to vary by subreach. Allowing the dispersion coefficient to vary by subreach only involved dimensioning the variable DQQ by branch and subreach in the model rather than just by branch. When the dispersion coefficient was allowed to vary by subreach, however, the input format needed to be modified. The input format for BLTM is described in Jobson and Schoellhamer (1987, p. 8-10 and Appendix A). The dispersion factor was removed from the first card (line) of data set 5 (Branch Information) and placed on the second card, which defines subreach specific information. The junction numbers at the upstream and downstream ends of the branch and the initial number of parcels per subreach are moved seven columns to the left on the first card. The subreach value of the dispersion coefficient is added as the third field on card two and the initial concentrations begin in field four rather than three. This means that there is only room for 7 constituent concentrations on this card rather than 8, and the third card of this data set must contain the initial concentrations of constituents 8 through 18 rather than 9 through 19. The dispersion factor is input in an F7.3 format.

The dispersion factor that is input for each subreach is output in the "bltm.out" file on a line by itself immediately following the information giving the location of the subreach and initial flow conditions.

Time-Dependent Data System (TDDS)

At the time the BLTM model was documented, it was believed that the BRANCH flow model (Schaffranek and others, 1981) would be the model most commonly used to provide hydraulic information. Soon after the documentation was published, the DAFLOW model (Jobson, 1989) was developed. The DAFLOW is much simpler to apply and can be used with ease for upland streams and rivers where the BRANCH model tends to be unstable. As a result, TDDS, developed for use with the BRANCH model, was seldom used. Because this routine increased the size of the model significantly and made the code harder to follow, this capability was removed from the model. Basically this eliminates the need to link the model to the DTDDS subroutine as well as the need for input data sets 6, 7, 8, 9, and 10. BLTM can still be used with BRANCH, or any other flow model, but the interface is through the file "bltm.flw", not the TDDS data system.

Accuracy criteria

The BLTM model solves many equations by iteration, so a criteria is needed to determine when the solution has converged. In addition, the Lagrangian solution scheme involves routing parcels (volumes) of water that can decrease in size by diversions to become insignificantly small. Originally the model had a fixed accuracy criteria to determine when to stop iterations or disregard a small water parcel. As the model was applied to systems that varied in size through many orders of magnitude, it became desirable to input an accuracy criteria that sets the scale of the system. The code was modified to query the user for an accuracy criteria (QI). This should be considered the minimum flow of interest because the model assumes any flow of less than this amount is zero. The model also assumes any volume of water that is smaller than this flow times the time-step size (DT) is insignificant. If a parcel of water becomes smaller than $QI \cdot DT$, it will be combined with another parcel and no longer tracked individually. The default value of QI is set as $1 \text{ ft}^3/\text{s}$ in the English system or $1 \text{ m}^3/\text{s}$ in the metric system.

Parameter Statements

The model was originally dimensioned to allow for a fixed number of branches, grids per branch, constituents, parcels per branch, and junctions. It is often desirable to change the dimension statements to customize the model to a particular problem. The arrays with dimensions that may need to be changed are now dimensioned with parameters. These parameters are defined in a single file, "params.inc", which is included in the subroutines by means of the INCLUDE statement (a common Fortran77 extension and a feature of Fortran 90). Defining the parameters in a single file ensures that the array dimensions are consistent in all subroutines. After modifying a parameter, the programs must be recompiled. A typical "params.inc" file follows:

```
INTEGER NOBR, NOSC, NOSH, NOCO, NOPR, NOCP, NOTS
C
C PARAMETER ( NOBR=15, NOSC=15, NOSH=300)
C PARAMETER ( NOCO=10, NOPR=150, NOCP=4000, NOTS=500)
C
C + + + PARAMETER DEFINITIONS + + +
C NOBR - Maximum number of branches allowed in model
C NOSC - Maximum number of cross sections (grids) allowed in branch
C NOSH - Maximum number of shocks allowed in branch
C          (NOSH should be at least 4 times NOSC)
C NOCO - Maximum number of constituents allowed
C NOPR - Maximum number of parcels allowed in branch
C          (NOPR should be at least 20 + 2 times NOSC)
C NOCP - Maximum number of computed or observed points
C NOTS - Maximum number of time steps (flwopt only)
```


DAFLOW/BRANCH Input

As mentioned above, when BLTM was written, it was anticipated that the BRANCH model would be used to supply the hydraulic input. The BRANCH model output contains the instantaneous river and tributary discharge at the end of the time step, 0, 1, 2, The cross-sectional area and top width are considered to be instantaneous values representative of the cross section at the grid point. The BLTM model, on the other hand, requires the values of discharge (both river and tributary) to be averaged over the time step. It also assumes the cross-sectional area and top width represent reach-averaged values at the end of the time step. The original BLTM code averaged the discharges at the beginning and end of the time step to provide a time-averaged value. It also averaged the areas and top widths at the cross sections for each end of the subreach to estimate the reach-averaged values of these variables.

The DAFLOW model outputs the time-step-averaged values of discharge and reach-averaged values of cross-sectional area and top width, which eliminated the need for averaging inside the BLTM program. The code was modified, therefore, to accept either type of input data; and the code ITDDS was changed from indicating the use of the TDDS data base to a code indicating whether or not averaging of hydraulic data was needed in the program. That is, if ITDDS = 0, the model assumes the DAFLOW type of output is read; if ITDDS = 1, it assumes the BRANCH type of output is read. The variable ITDDS is read just like the value in the original documentation.

The Subroutine QUAL2E

Purpose

The stream water-quality model, QUAL2E, developed by EPA, is widely used for waste load allocation, discharge permit determinations, and other conventional pollutant evaluations. The EPA-QUAL2E model has a number of limitations, such as the assumption that stream reaches must have uniform hydraulics, generally steady flow must be assumed, computational elements must be uniformly spaced, and it is generally difficult to modify the reaction kinetics to match special situations. The BLTM model eliminates or reduces these limitations while supplying the reaction kinetics shown in figure 4, which are identical to those used by the EPA-QUAL2E code. It is a fully dynamic model in that both flow and water-quality conditions are assumed to vary with time and space. By linking the QUAL2E subroutine to the BLTM transport model, the user gets the benefit of a fully dynamic model that simulates the EPA-QUAL2E reaction kinetics but also provides the very accurate dispersion and advection calculations generally only available in a Lagrangian type of transport model. The report by Bowie and others (1985) should be consulted for further details on the reaction kinetics and rate constants.

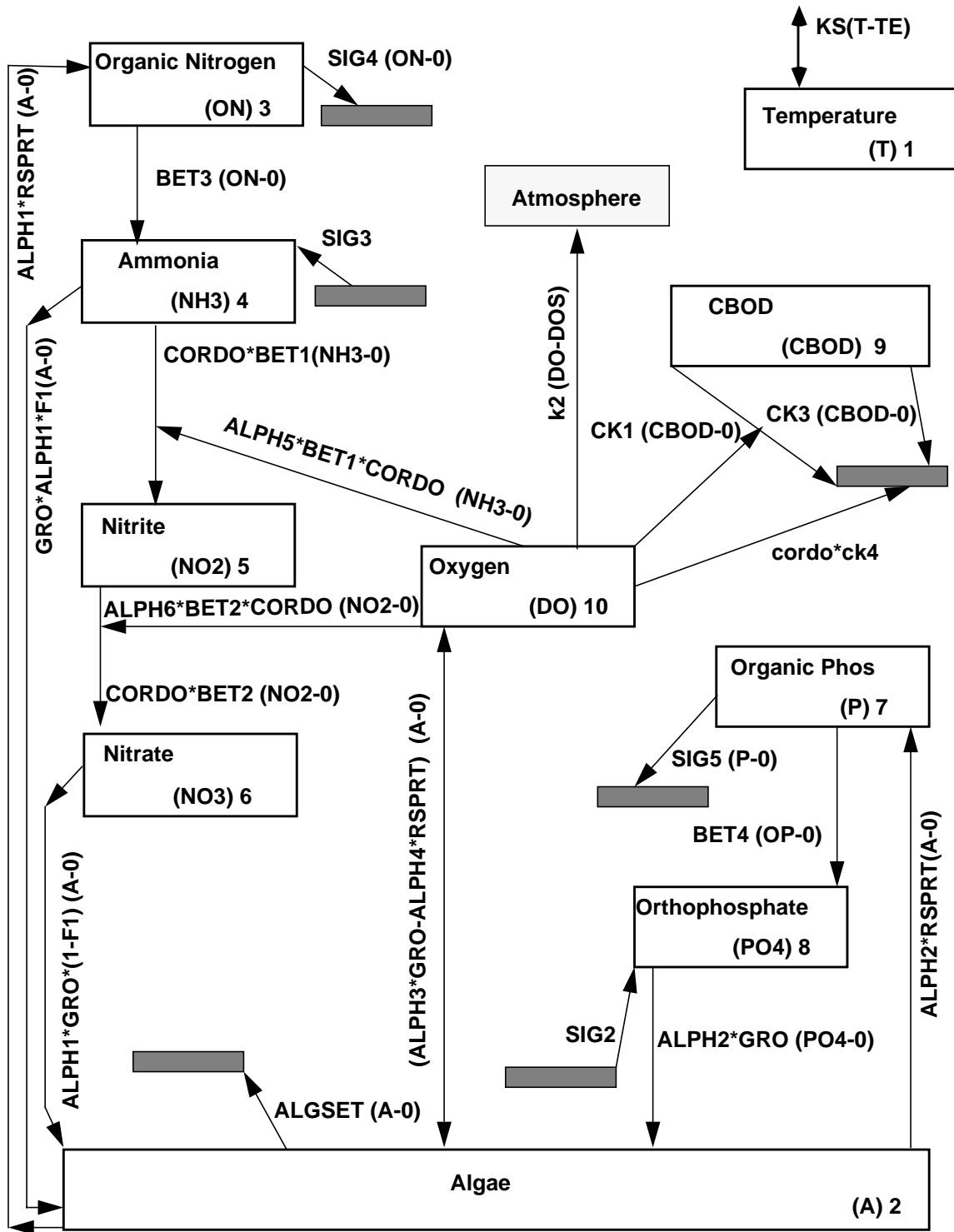


Figure 4. Schematic model of the QUAL2E reaction kinetics.

Differences Between BLTM-QUAL2E and the EPA Code

The BLTM model linked to the QUAL2E reaction kinetics subroutine is different from the EPA code as described below.

The linked BLTM-QUAL2E code, called QBLTM, allows the flow to be input in either the foot-second system or the meter-second system but the input to the QUAL2E subroutine ("qual2e.in") must be in the specified units. Generally this requires concentrations to be expressed as milligram per liter, rate constants to be in units of per day, source terms to be milligram of input per square foot per day, extinction coefficients to be in units of per foot, temperatures to be in degree Celsius, and solar radiation and light limitation constants to be calorie/square centimeter/minute (Langley/minute).

The BLTM code allows the effect of each individual reaction process on the change in concentration of each fluid parcel to be tabulated. This information is very useful in calibrating the model and in identifying which reactions are most important to the predicted concentration at any point in space or time.

The equations to compute the reaeration caused by dams and weirs are not included in the BLTM-QUAL2E code.

Because the model is expected to be used in the fully dynamic mode, there are no options for estimating the effective daily-averaged radiation values. It is assumed that the time step will be short enough that these averaging routines are not necessary or that the incoming radiation values are averaged before input to BLTM.

The QUAL2E subroutine contains a slightly different temperature routine than contained in the EPA-QUAL2E code so the temperature routine used by BLTM-QUAL2E is outlined below. The input to the temperature routine is equilibrium temperature, and wind speed, just as in the EPA model. The equilibrium temperature can be computed in any way the user chooses but a program to estimate its value, based on meteorologic data commonly available at airport weather stations, is included in this document. The heat exchange coefficient is determined as outlined below.

Applying the principle of conservation of thermal energy to a one-dimensional open channel, the conservation equation becomes:

$$\frac{dT}{dt} + U \cdot \frac{dT}{dx} - \left(D_x \cdot \frac{d^2T}{dx^2} \right) = \frac{H_t \cdot W}{C_p \cdot \rho \cdot A}, \quad (29)$$

where T = cross-sectional average water temperature, t = time, U = stream velocity, x = longitudinal coordinate, A = cross-sectional area, D_x = longitudinal dispersion coefficient, H_t = flux of thermal energy from the air to the water, W = top width of the channel, C_p = specific heat of water at constant pressure, and ρ = density of water.

The term on the right side of equation 29 represents the rate of change of water temperature due to exchange of energy between the water and atmosphere. If the equilibrium temperature is known, the net surface heat exchange can be approximated from the equation:

$$H_t = K \cdot (T - T_e) , \quad (30)$$

where T_e = equilibrium temperature; and K = the kinetic surface exchange coefficient, which is the slope of the curve of H_t vs. T , as shown in figure 3. The value of the surface exchange coefficient is determined as the negative of the derivative, with respect to T , of the sum of equations 2, 6, and 7 or:

$$K = -\epsilon \cdot \sigma \cdot (T + 273.18)^3 - \rho \cdot L \cdot \psi \cdot (e_{op} - \gamma) , \quad (31)$$

where e_{op} = slope of the saturation vapor pressure curve with respect to temperature, obtained by differentiating equation 4 with respect to T , or from an empirical estimating equation, and the energy exchange caused by rainfall (equation 8) is ignored. As can be seen from equation 31, the surface exchange coefficient is only a function of the water temperature and wind speed, furthermore the dependence on wind speed is fairly weak (fig. 2). If the equilibrium temperature can be estimated, therefore, the value of the net surface heat exchange can be computed with little meteorologic data.

To simplify computations, the slope of the saturation vapor pressure curve, e_{op} , is computed from the empirical equation:

$$e_{op} = 1.1532 \times 10^{11} \cdot \frac{\exp(-4271.1 / (T + 242.63))}{(T + 242.63)^2} , \quad (32)$$

where e_{op} is given in kilopascals per degree Celsius, and the temperature is input in Celsius degrees. When compared to slopes determined by subtracting values at whole degrees, obtained from published vapor pressures (Hodgman, 1960), the accuracy of equation 32 is within 1 percent for the range of 0.5 to 39.5 degrees. Within the range of 2.5 to 34.5 degrees, the accuracy is within 0.25 percent. Generally, improved accuracy could be obtained by using the derivative of equation 4, but the small increase in accuracy was judged not to merit the increased complexity of the equation. The EPA-QUAL2E code uses different, less accurate, empirical equations for the estimating of these values.

Input Data and Format

The QUAL2E subroutine requires an input file called "qual2e.in", which is described in detail below. The input file can be generated by use of a full screen editor or by use of the program called BQUAL2E. The format of the file "qual2e.in" is as follows:

- (1) The first line contains up to 80 characters of text, which can be used as identification. The model prints this information as identification in the output file.
- (2) The second line also contains text information defining the two parameters in the wind function, which are contained on the line that follows. The parameters are defined as:
 - A1 Constant in wind function of equation 5 [mm/day kPa];
 - B1 Mass transfer coefficient of equation 5 [mm/day/kPa/(m/s)].
- (3) The third line contains the two parameters to be used in the wind function (equation 5). The two parameters can be placed anywhere on the line but A1 must proceed B1 and the two numbers must be separated by at least one blank space.
- (4) Contains header information listing the Fortran names of the ten coefficients that are contained on the next line. The Fortran names of the coefficients are chosen to be similar to those used in the EPA-QUAL2E model (Brown and Barnwell, 1987). The variables, all of which have a single value for the entire domain, are listed and defined below:
 - ALPH0 Conversion factor, μg Chlorophyll-A/mg Algae;
 - ALPH1 Fraction of algal biomass that is nitrogen, mg-N/mg-Algae;
 - ALPH2 Fraction of algae biomass that is phosphorus, mg-P/mg-Algae;
 - ALPH3 Oxygen production per unit of algal growth, mg-O/mg-Algae;
 - ALPH4 Oxygen uptake per unit of algae expired, mg-O/mg-Algae;
 - ALPH5 Oxygen uptake per unit of NH_3 oxidation, mg-O/mg-N;
 - ALPH6 Oxygen uptake per unit of NO_2 oxidation, mg-O/mg-N;
 - GROMAX Maximum specific growth rate of algae, per day;
 - IGRO Growth rate option,
 - 1. = multiplicative,
 - 2. = limiting nutrient,
 - 3. = Harmonic mean;
 - RSPRT Algal respiration rate, per day.
- (5) Contains the ten coefficients, in the order listed above, with each variable separated by at least one blank space. Any format can be used for the coefficients.

- (6) Contains header information listing the Fortran names of the nine coefficients that are given on the next line. Except for the shading coefficients, the Fortran names of the coefficients are chosen to be as similar as possible to those used in the EPA-QUAL2E code. The variables, all of which have a single value for the entire domain, are listed and defined below:

| | |
|-------|--|
| LFO | Light function option, 1.= half saturation, 2.= Smith's function, 3.= Steel's equation; |
| CKL | Light constant, $\text{cal/cm}^2/\text{min}$) = Langley/min, LFO =1, CKL = half saturation coefficient, LFO =2, CKL = light intensity at 71% max growth rate, LFO =3, CKL = light intensity at max growth rate; |
| CKN | Nitrogen half-saturation constant for algae, mg/L; |
| CKP | Phosphorus half-saturation constant for algae, mg/L; |
| SHAD0 | Non-algal portion of light extinction coefficient, per ft; |
| SHAD1 | Linear algal self shading coefficient; |
| SHAD2 | Nonlinear algal self shading coefficient; |
| PN | Preference factor for ammonia nitrogen (0-1.0); |
| K2O | Option for K_2 (reaeration coefficient input), 1 = read as input, 2 = Churchill, Elmore, and Buckingham (1962), 3 = O'Connor and Dobbins (1958), 4 = Owens et al (1964), 5 = Thackston and Krenkel (1966), 6 = Langbien and Durum (1967), 7 = power function equation of flow, 8 = Tsivoglou and Wallace (1972). |

- (7) Contains the nine coefficients, in the order listed above, with each variable separated by at least one blank space. Any format can be used for the coefficients.
- (8) Contains header information listing the Fortran names of the seven coefficients that are given on the next lines. These coefficients are variable between subreaches so there will be one line for each subreach of the model. The first two numbers will identify the branch and subreach (grid) number for the data contained on that line. The branches and subreaches can be placed in any order because the location for the data is contained on the line, but there must be one line for each subreach in the model. The variables are listed and defined below:

| | |
|--------|---|
| BR | Branch for which the information applies; |
| GR | Subreach for which the information applies; |
| ALGSET | Local settling rate for algae, ft/day; |
| BET3 | Rate constant for ON to NH_3 transformation, per day; |
| SIG4 | Organic nitrogen settling rate, per day; |
| BET1 | Rate constant for biological oxidation of NH_3 to NO_2 , per day; |
| SIG3 | Benthos source rate for NH_3 , $\text{mg-N}/\text{ft}^2$ day; |
| BET2 | Rate constant for biological oxidation of NO_2 to NO_3 , per day; |
| BET4 | Organic phosphorus decay rate, per day. |

- (9) Contains the branch and subreach number followed by the seven coefficients, in the order listed above, with each variable separated by at least one blank space. Any format can be used.
- (10) Contains header information listing the Fortran names of the five to seven coefficients that are given on the next lines. These coefficients are variable between subreaches so there will be one line for each subreach of the model. The first two numbers will identify the branch and subreach (grid) number for the data contained on that line. The branches and subreaches can be placed in any order because the location for the data is contained on the line but there must be one line for each subreach in the model. The variables are listed and defined below:
- | | |
|------|---|
| BR | Branch for which the information applies; |
| GR | Subreach for which the information applies; |
| SIG5 | Organic phosphorus settling rate, per day; |
| SIG2 | Benthos source rate for dissolved P, mg-P/ft ² day; |
| CK1 | Carbonaceous CBOD decay rate, per day; |
| CK3 | Carbonaceous CBOD sink rate, per day; |
| CK4 | Benthos consumption of oxygen, mg-O/ft ² /day; |
| CK2 | Reaeration rate, per day for reaeration option 1, Manning's for reaeration option 5 or 8, Coefficient on Q for reaeration option 7, Not needed for reaeration option 2,3,4 or 6; |
| CB | Exponent on flow for reaeration option 7, not needed for any other reaeration option. |
- (11) Contains the branch and subreach number followed by the five to seven coefficients, in the order listed above, with each variable separated by at least one blank space. Any format may be used.
- (12) Contains header information listing the Fortran names of the three input variables that vary with time that are given on the next lines. One line of data is needed for each time step in the model. The first number is ignored by the model but it is convenient to use this to identify either the time or the time-step number. The three variables are listed and defined below:
- | | |
|-------|---|
| Time | Can be any number because it is ignored in the model; however, there must be a number here; |
| TE | Equilibrium temperature, degrees Celsius; |
| V | Wind speed, meter/second; |
| SONET | Light intensity, cal/cm ² /min = Langley/min. |
- (13) Contains the time, equilibrium temperature, wind speed, and solar radiation, in that order, with each variable separated by at least one blank space. Any format may be used and the magnitude of the number in the time column is not important.

LEVEL 5— PROGRAMS TO PLOT CONCENTRATION AS A FUNCTION OF TIME OR DISTANCE (CTPLT, CXPLT)

Postprocessor program CTPLT reads parcel information from the file "parcel.out" and plots a concentration as a function of time for any river mile within the modeled system. This program is essentially unchanged since it was described in the original documentation, so it will be discussed only briefly. The program may also read a file called "obs" containing a table of times and concentrations and plot these concentrations as observed values for comparison with the computed values. If the option is selected to plot observed values, the program computes the mean and root-mean-square (RMS) error between the computed and observed values. The input file "obs" is in the standard format, containing two lines of text at the beginning and two or more columns of data separated by at least one space. The first column is assumed to be time measured from midnight of the day that modeling was started. The second column is assumed to be concentration at the time indicated in the first column and all other columns are ignored. Results are written to a file called "plt.out", which contains three sections. The first section contains the computed concentrations for all time steps, the second contains the observed concentrations, and the last lists the mean and RMS error in the observed points. The output file is in a format that can be easily imported into a more robust plot package to generate high-quality graphics.

The program CXPLT reads information from the files "parcel.out" and "*bltm.in*" to plot the variation of concentration as a function of distance along the channel for any specified time step. The concentration in any number of branches can be plotted as a continuous profile. This program is also essentially unchanged since it was first documented.

EXAMPLE APPLICATION OF QUAL2E REACTION KINETICS TO THE CHATTAHOOCHEE RIVER

The purpose of this example is to demonstrate the use of the programs documented in this report by applying the BLTM with the QUAL2E reaction kinetics to water quality in the Chattahoochee River below Atlanta, Ga. The constituents modeled include temperature (1), algae (2), organic nitrogen (3), ammonia (4), nitrite (5), nitrate (6), organic phosphorus (7), dissolved phosphorus (8), carbonaceous CBOD (9), and dissolved oxygen (10). The reach to be modeled extends from the Route I-280 bridge in Atlanta to Fairburn, which is about 17 miles downstream. A period of 48 hours, which starts at 1800 hours on May 31, 1977, will be simulated. The Route I-280 bridge is just downstream of the Atkinson and McDonough power plants, which use the river water for cooling. The Clayton wastewater treatment facility also is just a short distance upstream from the bridge, and its effluent dominates the water quality in this reach of the river. Data necessary to model the water quality have been published in Jobson (1985).

The river flow at the Route I-280 bridge varied from a low of 1,210 ft³/s to a maximum of 1,300 ft³/s during the model period, but for simplicity, all flows will be assumed to be constant at the values shown in table 1. The slope of this reach of the river is about 0.000309 ft/ft (Faye and others, 1979, p. 9).

Table 1. Flows in the Chattahoochee River on June 1, 1977.

| Grid | Site name | Initial values | | | |
|------|------------------|--------------------|-----------------------------------|---------------------------------------|-----------------|
| | | Location (mile) | Tributary (ft ³ /s) | River Flow (ft ³ /s) | Width (feet) |
| 1 | Route I-280 | 4.20 | | 1,250 | 250 |
| 2 | Nickajack Creek | 7.84 | 28 | 1,278 | |
| 3 | South Cobb | 8.69 | 14 | 1,292 | |
| 4 | Utoy Creek | 11.40 | 29 | 1,321 | 230 |
| 5 | Sweetwater Creek | 14.39 | 155 | 1,476 | |
| 6 | Camp Creek | 19.43 | 49 | 1,525 | 240 |
| 7 | Fairburn | 21.18 | | | 260 |

Although the flows are assumed to be constant for purposes of this example, the modeling system assumes all flows are unsteady; therefore, the first step is to model the flow. This can be done by using the DAFLOW model documented by Jobson (1989). Reasonable hydraulic geometry coefficients for use in this model estimate the flow area by the equation:

$$A = 190 + 4.52 \cdot Q^{0.70},$$

where A = cross sectional flow area, in square foot and Q = discharge, in cubic foot per second. Likewise, the top width is estimated by the equation:

$$W = 31 \cdot Q^{0.26},$$

where W = top width of the river, in feet. The coefficients in these two equations were obtained by calibrating the flow model to the unsteady flows obtained in 1976 (Jobson, 1985) and to time-of-travel data published by Nordin and Sabol (1974). Table 2 is a listing of the input file for DAFLOW, "flow.in." This file also is used by the program BBLTM to create the input file "bltm.in" for use by the transport model (fig. 1).

Table 2. Input file "flow.in" for the DAFLOW model of the Chattahoochee River.

```

Input file for the DAFLOW model of the Chattahoochee River, Rte 280-Fairburn
No. of Branches          1 *
Internal Junctions       0 *
Time Steps Modeled      48 *
Model Starts             18 *   Time steps after midnight.
Output Given Every      1 *   Time Steps in 'flow.out'
0=Metric,1=English      1 *
Time Step Size          1.000 *   Hours.
Peak Discharge          50000. *
Branch 1 has 7 xsects & routes 1.00 of flow at JNCT 1 To JNCT 2
Grd  R Mile  IOUT Disch   A1    A2    AO    Slope      W1    W2
 1   4.200   0    1250.   4.52  0.700  190.  0.309E-03  31.0  0.260
 2   7.840   0    1278.   4.52  0.700  190.  0.309E-03  31.0  0.260
 3   8.690   0    1292.   4.52  0.700  190.  0.309E-03  31.0  0.260
 4   11.40   0    1321.   4.52  0.700  190.  0.309E-03  31.0  0.260
 5   14.39   0    1476.   4.52  0.700  190.  0.309E-03  31.0  0.260
 6   19.43   0    1509.   4.52  0.700  190.  0.309E-03  31.0  0.260
 7   21.18   1
for Time 1 NBC= 6 *
Branch 1 Grid 1 Q= 1250.0 *
Branch 1 Grid 2 Q= 28.000 *
Branch 1 Grid 3 Q= 14.000 *
Branch 1 Grid 4 Q= 29.000 *
Branch 1 Grid 5 Q= 155.00 *
Branch 1 Grid 6 Q= 33.000 *
for Time 2 NBC= 0 *
for Time 3 NBC= 0 *
.
.
.
for Time 47 NBC= 0 *
for Time 48 NBC= 0 *

```

The flow model prints two files—one of which, "bltm.flw" (see fig 1), is input for the transport model. Table 3 contains a listing of this file for time-step zero, which is the initial condition. Because the flow is assumed to be steady, the file contains identical numbers for all other time steps. The columns are defined as follows: "J," time-step number; "N," branch number; "I," grid or subreach number; "Discharge," river discharge just downstream of grid point, in cubic foot per second; "Area," average cross-sectional flow area for the subreach, in square foot; "Top Width," average top width of water for the subreach, in feet; and "Trib flow," tributary inflow at the grid point to the river, in cubic foot per second. Subreach 1 extends from grid 1 to grid 2.

Table 3. Listing of the hydraulic data contained in the file "bltm.flw" for one time step.

| J | N | I | Discharge | Area | Top Width | Trib flow |
|---|---|---|-------------|-------------|-------------|-------------|
| 0 | 1 | 1 | 0.12500E+04 | 0.85524E+03 | 0.19795E+03 | 0.00000E+00 |
| 0 | 1 | 2 | 0.12780E+04 | 0.86563E+03 | 0.19909E+03 | 0.28000E+02 |
| 0 | 1 | 3 | 0.12920E+04 | 0.87080E+03 | 0.19966E+03 | 0.14000E+02 |
| 0 | 1 | 4 | 0.13210E+04 | 0.88147E+03 | 0.20082E+03 | 0.29000E+02 |
| 0 | 1 | 5 | 0.14760E+04 | 0.93731E+03 | 0.20669E+03 | 0.15500E+03 |
| 0 | 1 | 6 | 0.15090E+04 | 0.94896E+03 | 0.20788E+03 | 0.33000E+02 |
| 0 | 1 | 7 | 0.15090E+04 | | | |

With the files "flow.in" and "bltm.flw" created, the hydraulics of the system are defined, and the transport model can be operated.

The next step is to build the file "bltm.in" shown in figure 1. This file contains geometry information, as well as initial and boundary conditions, for each constituent. The program BBLTM, which is designed to help build the input file "bltm.in," obtains the geometry information from the file "flow.in," the initial conditions from the keyboard, and the boundary conditions from either the keyboard or from the file "bc." Any number of boundary conditions can be entered from the keyboard, but the boundary conditions for only one grid can be obtained in the file "bc" during any run of BBLTM. If boundary conditions for two or more grids are to be input from a file, then the program BBLTM must be run for each new boundary condition. This procedure will be illustrated below. Most boundary conditions for this example are assumed to be constant at the initial values shown in table 4. Because only 48 time steps are modeled, the constant boundary conditions are entered from the keyboard.

Table 4. Initial water quality in the Chattahoochee River at 1800 hours on May 31, 1977.

| Grid | Site | Temp | A | ON | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO |
|------|---------------|---------------------------------------|---|------|------|------|------|------|------|------|-----|
| 1 | Route 280 | | | | | | | | | | |
| | Chattahoochee | 30.6 | 0 | 1.1 | 2.47 | 0.04 | 0.40 | 0.23 | 0.44 | 16.5 | 8.7 |
| 2 | Nickajack Crk | 21.5 | 0 | 1.7 | 1.5 | 0.02 | 0.50 | 0.4 | 0.7 | 28.7 | 7.4 |
| | Chattahoochee | 29.9 | 0 | 0.6 | 1.6 | 0.01 | 0.46 | 0.17 | 0.17 | 17.0 | 7.4 |
| 3 | S Cobb Creek | 20.8 | 0 | 8.3 | 13.0 | 0.08 | .04 | 2.9 | 6.0 | 86.3 | 0.6 |
| | Chattahoochee | 29.3 | 0 | 0.6 | 1.6 | 0.01 | 0.60 | 0.17 | 0.17 | 17.0 | 7.9 |
| 4 | Utoy Creek | Variable with time, input from a file | | | | | | | | | |
| | Chattahoochee | 27.6 | 0 | 0.83 | 1.3 | 0.02 | 0.61 | 0.16 | 0.35 | 16.7 | 6.9 |
| 5 | Sweetwater Cr | 21.7 | 0 | 0.47 | 0.05 | 0.01 | 0.28 | 0.04 | 0 | 5.1 | 7.7 |
| | Chattahoochee | 26.1 | 0 | 0.63 | 1.1 | 0.05 | 0.56 | 0.12 | 0.35 | 17.0 | 6.8 |
| 6 | Camp Creek | 20.9 | 0 | 0.48 | 1.2 | 0.03 | 0.8 | 0.05 | 1.1 | 5.5 | 7.4 |
| | Chattahoochee | 26.2 | 0 | 0.58 | 1.0 | 0.05 | 0.65 | 0.10 | 0.38 | 17.2 | 6.8 |
| 7 | Fairburn | | | | | | | | | | |

The boundary conditions at Route I-280 and at the Utoy Creek, grid 4, are assumed to be variable with time so they will be input from a file "bc." The boundary condition at Route I-280 will be added in the first run of BBLM. Table 5 contains boundary conditions at Route I-280 in a format acceptable to the program BBLTM; that is, two lines of text at the top with a column of times, which are ignored, and a column for each constituent separated by at least one space. Two columns in table 5, "Alga" and "CBOD," contain all zeros. No data are available for algal concentrations. Because field observations indicated that little was present in the river the concentration will be assumed to be zero for this example. The CBOD column will be added to the table to illustrate the use of the programs INTRP and MRG.

Table 5. Boundary conditions (excepting CBOD) at the Route I-280 bridge starting at hour 18.5 on May 31, 1977.

| Chattahoochee River observed data at Route I-280 starting on May 31, 1977 | | | | | | | | | | |
|---|-------|------|------|------|------|------|------|------|------|------|
| Time | Temp | Alga | ON | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO |
| 18.50 | 29.62 | 0.00 | 0.93 | 2.50 | 0.04 | 0.32 | 0.22 | 0.55 | 0.00 | 8.68 |
| 19.50 | 29.86 | 0.00 | 0.78 | 2.50 | 0.04 | 0.35 | 0.16 | 0.48 | 0.00 | 8.63 |
| 20.50 | 29.94 | 0.00 | 0.74 | 2.46 | 0.04 | 0.37 | 0.15 | 0.45 | 0.00 | 8.60 |
| . | . | . | . | . | . | . | . | . | . | . |
| 63.50 | 29.36 | 0.00 | 0.63 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 0.00 | 7.90 |
| 64.50 | 29.25 | 0.00 | 0.65 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 0.00 | 7.90 |
| 65.50 | 29.13 | 0.00 | 0.67 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 0.00 | 7.90 |

Table 6 contains the observed data for CBOD at the Route I-280 bridge in a format that is acceptable for INTRP; that is, two lines of text followed by a time column and a column of data with data separated by at least one space.

Table 6. Boundary conditions for CBOD at the Route I-280 bridge starting at hour 17.5 on May 31, 1977.

| Hour | Oxygen demand, biochemical Ultimate Carbonaceous (mg/L) CBOD (parameter code = 00320) |
|-------|--|
| 17.50 | 20.00 |
| 19.00 | 16.00 |
| 21.08 | 18.00 |
| 25.25 | 14.00 |
| 27.83 | 15.00 |
| 30.00 | 3.60 |
| 33.00 | 15.00 |
| 36.00 | 9.60 |
| 40.00 | 25.00 |
| 40.5 | 25.0 Interpolated from Route 139 data |
| 42.0 | 22.0 Interpolated from Route 139 data |
| 43.00 | 18.00 |
| 46.00 | 14.00 |
| 47.50 | 16.00 |
| 50.00 | 15.00 |
| 52.75 | 16.00 |
| 58.25 | 11.00 |
| 66.6 | 11.0 assumed value |

Placing the data in table 6 in a file called "in" and executing the program INTRP would read file "in" and write a file "bc" with an output as shown in table 7. Notice that the program INTRP has interpolated between observed points to generate input concentrations every hour, the time-step size in the model, starting at hour 18.5, the mid-point of the first time step. The program BLTM assumes that the boundary conditions represent the average input concentrations during the time step; this is approximated by interpolating to the middle of the time step. When the program INTRP is executed to generate the output shown in table 7, the operator should enter a "starting value of x" of 18.5, a "value of DX," the interval between interpolated points of 1 hour, and the "number of points to be interpolated" of 48. The "transport format" should be selected for the output. The first two lines of the input file have been written as the first two lines of the output file without modification.

Table 7. Output of the program INTRP when used to interpolate CBOD values to 1-hour intervals.

| Oxygen demand, biochemical Ultimate Carbonaceous (mg/L) | |
|---|-------------------------------|
| Hour | CBOD (parameter code = 00320) |
| 18.50 | 17.33 |
| 19.50 | 16.48 |
| 20.50 | 17.44 |
| 21.50 | 17.60 |
| 22.50 | 16.64 |
| 23.50 | 15.68 |
| . | |
| . | |
| . | |
| 63.50 | 11.00 |
| 64.50 | 11.00 |
| 65.50 | 11.00 |

The next step is to merge the second column of table 7 with the CBOD column of table 5, which is accomplished with either a full screen editor or by using the program MRG. To use the program MRG, the data in table 5 are placed in a file called "old.bc," the data in table 7 are placed in a file called "in," and the program MRG is executed. When executing MRG, the operator should enter "7" as the output format option, "10" as the "number of data columns in "old.bc," and "9" as the "column no. (excluding time) to be changed." Once this is completed, the output file from MRG, the file "bc," should be identical to the data in table 8.

Table 8. Complete boundary conditions at the Route I-280 bridge starting at hour 18.5 on May 31, 1977.

| Chattahoochee River observed data at Route I-280 starting on May 31, 1977 | | | | | | | | | | |
|---|-------|-------|------|------|------|------|------|------|-------|------|
| Time | Temp | Algae | ON | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO |
| 18.50 | 29.62 | 0.00 | 0.93 | 2.50 | 0.04 | 0.32 | 0.22 | 0.55 | 17.33 | 8.68 |
| 19.50 | 29.86 | 0.00 | 0.78 | 2.50 | 0.04 | 0.35 | 0.16 | 0.48 | 16.48 | 8.63 |
| 20.50 | 29.94 | 0.00 | 0.74 | 2.46 | 0.04 | 0.37 | 0.15 | 0.45 | 17.44 | 8.60 |
| 21.50 | 29.80 | 0.00 | 0.84 | 2.36 | 0.04 | 0.36 | 0.19 | 0.46 | 17.60 | 8.60 |
| 22.50 | 28.65 | 0.00 | 0.93 | 2.27 | 0.04 | 0.35 | 0.19 | 0.47 | 16.64 | 8.60 |
| 23.50 | 27.50 | 0.00 | 1.03 | 2.17 | 0.04 | 0.35 | 0.20 | 0.48 | 15.68 | 8.60 |
| 24.50 | 26.90 | 0.00 | 1.09 | 2.08 | 0.04 | 0.34 | 0.21 | 0.49 | 14.72 | 8.28 |
| 25.50 | 26.52 | 0.00 | 1.05 | 2.00 | 0.04 | 0.35 | 0.21 | 0.50 | 14.10 | 8.20 |
| 26.50 | 26.13 | 0.00 | 1.01 | 1.93 | 0.03 | 0.37 | 0.22 | 0.52 | 14.48 | 8.13 |
| 27.50 | 25.75 | 0.00 | 0.94 | 1.84 | 0.03 | 0.38 | 0.20 | 0.49 | 14.87 | 8.07 |
| 28.50 | 25.38 | 0.00 | 0.85 | 1.75 | 0.04 | 0.39 | 0.16 | 0.44 | 11.48 | 8.02 |
| 29.50 | 25.50 | 0.00 | 0.77 | 1.65 | 0.04 | 0.40 | 0.13 | 0.38 | 6.23 | 7.93 |
| 30.50 | 26.10 | 0.00 | 0.70 | 1.55 | 0.04 | 0.39 | 0.12 | 0.31 | 5.50 | 7.80 |
| 31.50 | 26.70 | 0.00 | 0.63 | 1.45 | 0.03 | 0.39 | 0.11 | 0.24 | 9.30 | 7.80 |
| 32.50 | 27.08 | 0.00 | 0.62 | 1.40 | 0.03 | 0.39 | 0.10 | 0.20 | 13.10 | 7.80 |
| 33.50 | 27.25 | 0.00 | 0.65 | 1.40 | 0.03 | 0.39 | 0.11 | 0.17 | 14.10 | 7.80 |
| 34.50 | 27.42 | 0.00 | 0.68 | 1.40 | 0.03 | 0.40 | 0.12 | 0.15 | 12.30 | 7.80 |
| 35.50 | 27.67 | 0.00 | 0.83 | 1.45 | 0.03 | 0.40 | 0.19 | 0.16 | 10.50 | 7.83 |
| 36.50 | 28.00 | 0.00 | 1.10 | 1.55 | 0.04 | 0.39 | 0.32 | 0.19 | 11.53 | 7.90 |
| 37.50 | 28.33 | 0.00 | 1.50 | 1.65 | 0.04 | 0.39 | 0.45 | 0.23 | 15.38 | 7.97 |
| 38.50 | 28.60 | 0.00 | 3.00 | 1.45 | 0.05 | 0.38 | 0.56 | 0.40 | 19.23 | 8.20 |
| 39.50 | 28.94 | 0.00 | 2.60 | 1.30 | 0.05 | 0.37 | 0.56 | 0.62 | 23.08 | 8.77 |
| 40.50 | 29.43 | 0.00 | 1.80 | 1.50 | 0.05 | 0.37 | 0.53 | 0.64 | 25.00 | 9.50 |
| 41.50 | 29.33 | 0.00 | 1.60 | 1.70 | 0.04 | 0.37 | 0.46 | 0.65 | 23.00 | 9.41 |
| 42.50 | 29.24 | 0.00 | 1.50 | 1.90 | 0.04 | 0.37 | 0.37 | 0.67 | 20.00 | 9.32 |
| 43.50 | 29.14 | 0.00 | 1.40 | 2.10 | 0.04 | 0.37 | 0.28 | 0.69 | 17.33 | 9.23 |
| 44.50 | 29.05 | 0.00 | 0.80 | 2.30 | 0.04 | 0.37 | 0.19 | 0.70 | 16.00 | 9.14 |
| 45.50 | 28.83 | 0.00 | 0.63 | 2.30 | 0.04 | 0.38 | 0.13 | 0.70 | 14.67 | 8.97 |
| 46.50 | 28.50 | 0.00 | 0.70 | 2.10 | 0.04 | 0.39 | 0.10 | 0.68 | 14.67 | 8.70 |
| 47.50 | 27.50 | 0.00 | 0.74 | 2.14 | 0.04 | 0.37 | 0.11 | 0.68 | 16.00 | 8.66 |
| 48.50 | 26.50 | 0.00 | 0.78 | 2.18 | 0.04 | 0.36 | 0.12 | 0.68 | 15.60 | 8.62 |
| 49.50 | 25.82 | 0.00 | 0.80 | 2.16 | 0.04 | 0.35 | 0.14 | 0.67 | 15.20 | 8.58 |
| 50.50 | 25.45 | 0.00 | 0.80 | 2.09 | 0.04 | 0.36 | 0.17 | 0.64 | 15.18 | 8.55 |
| 51.50 | 25.09 | 0.00 | 0.80 | 2.02 | 0.04 | 0.36 | 0.20 | 0.61 | 15.55 | 8.51 |
| 52.50 | 25.27 | 0.00 | 0.76 | 1.93 | 0.04 | 0.36 | 0.19 | 0.54 | 15.91 | 8.42 |
| 53.50 | 25.64 | 0.00 | 0.70 | 1.84 | 0.04 | 0.37 | 0.17 | 0.46 | 15.32 | 8.31 |
| 54.50 | 26.00 | 0.00 | 0.65 | 1.75 | 0.04 | 0.38 | 0.16 | 0.39 | 14.41 | 8.20 |
| 55.50 | 26.36 | 0.00 | 0.60 | 1.66 | 0.03 | 0.38 | 0.13 | 0.31 | 13.50 | 8.09 |
| 56.50 | 26.73 | 0.00 | 0.54 | 1.57 | 0.03 | 0.39 | 0.11 | 0.23 | 12.59 | 7.98 |
| 57.50 | 27.15 | 0.00 | 0.51 | 1.50 | 0.03 | 0.39 | 0.10 | 0.17 | 11.68 | 7.90 |
| 58.50 | 27.76 | 0.00 | 0.53 | 1.50 | 0.03 | 0.39 | 0.10 | 0.16 | 11.00 | 7.90 |
| 59.50 | 28.38 | 0.00 | 0.55 | 1.50 | 0.04 | 0.39 | 0.09 | 0.16 | 11.00 | 7.90 |
| 60.50 | 28.99 | 0.00 | 0.57 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 11.00 | 7.90 |
| 61.50 | 29.60 | 0.00 | 0.59 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 11.00 | 7.90 |
| 62.50 | 29.48 | 0.00 | 0.61 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 11.00 | 7.90 |
| 63.50 | 29.36 | 0.00 | 0.63 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 11.00 | 7.90 |
| 64.50 | 29.25 | 0.00 | 0.65 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 11.00 | 7.90 |
| 65.50 | 29.13 | 0.00 | 0.67 | 1.50 | 0.04 | 0.39 | 0.09 | 0.15 | 11.00 | 7.90 |

With the data in table 8 in a file called "bc" and the data in table 1 in a file called "flow.in," the program BBLTM can be executed to generate an input file for QBLTM called "bltm.in." In addition to the data contained in the two files, the operator must enter additional information from the keyboard. Table 9 contains the list of queries generated by BBLTM and the responses needed for the example application. The responses to the queries will be explained in some detail following the table.

Following the steps in table 9, the first option is to select a new file because this is the first time this model application has been run. The program title will be printed as the first line in the file "bltm.out." The number of time steps from midnight until the start of the model and the number of time steps between printouts in the file "bltm.out" are read from the "flow.in" file. Because a time-concentration plot is to be produced later, results should be written to the file "parcel.out" for every time step (JPO=1). Ten constituents (NEQ) are modeled, and a minimum dispersive velocity (DQV) of 0.0 is selected because this is a riverine environment where zero flow velocities are not likely. The labels for each constituent are then entered along with the constituent number for which the reactions will be tracked (LR). For example, when LR is selected as "10" for dissolved oxygen (constituent 10), the variable PDC contains the integral:

$$PDC = \int K_{10,10} \cdot (DO - DO_{sat}) dt,$$

where $K_{10,10}$ = the reaeration coefficient, DO = the dissolved oxygen concentration, and DO_{sat} = the saturation value of dissolved oxygen. The equation is integrated from the time the water parcel enters the branch until the time of the printout. Consequently, the value of PDC in "bltm.out" is the amount of oxygen absorbed by the water parcel as a result of reaeration from the time it entered the branch until the time of the print out. However, if LR is selected as "9" for dissolved oxygen, then the value of PDC contains the integral:

$$PDC = \int K_{10,9} \cdot (CBOD - 0) dt,$$

where $K_{10,9}$ = the rate of oxygen consumption by CBOD decay, CBOD = the CBOD concentration (constituent 9) in the water parcel, and PDC = the total oxygen consumed by CBOD since the water entered the branch.

Table 9. Queries generated by the program BBLTM and responses needed in this example application.

| Query | Response |
|---|-------------------------------|
| Enter 0 to create new file, 1 to edit existing file- | 0 |
| Input file for the DAFLOW model of Chattahoochee River Rte 280-Fairburn Enter new title (do not exceed 80) characters | Chattahoochee example problem |
| Enter number of time steps between outputs in "parcel.out- To select default enter any letter except d or e, Default=1, JPO= | 1 |
| Enter number of constituents to be modeled- | 10 |
| Enter minimum dispersive velocity, Default=0.0, DQV= | 0 |
| Enter label for constituent 1 (4 char max)- | Temp |
| Enter constituent no. to be tracked by PDC, Default= 1 LR= | 1 |
| . | |
| . | |
| Enter label for constituent 10 (4 char max)- | DO |
| Enter constituent no. to be tracked by PDC, Default= 10 LR= | 10 |
| For branch 1 enter the following: Initial number of parcels in each subreach, Default= 1 IPPR = | 3 |
| For each cross section (grid) enter the following: Enter the following for branch 1 Grid 1 Dispersion factor = dis coef/(U*U*DT), Default= 0.2000000, DQQ = | 0.06 |
| Initial concentration for subreach 1 Temp Default= 0.0000000E+00, Value = | 30.6 |
| . | |
| . | |
| DO Default= 0.0000000E+00, Value = | 8.7 |
| . | |
| . | |
| Enter the following for branch 1 Grid 6 Dispersion factor = dis coef/(U*U*DT), Default= 5.9999999E-02 DQQ = | x |
| Initial concentration for subreach 6 Temp Default= 26.00000 , Value = | 26.2 |
| . | |
| . | |
| DO Default= 6.000000 , Value = | 6.8 |
| For branch 1 Enter an output GRID (enter q to quit) | 3 |

Table 9. Queries generated by the program BBLTM and responses needed in this example application (continued).

| Query | Response |
|---|----------|
| Enter an output GRID (enter q to quit) | 7 |
| Enter an output GRID (enter q to quit) | q |
| Enter 1 to read a boundary condition from file "bc"- Enter 0 or n otherwise | 1 |
| Enter BRANCH of boundary condition in file "bc"- | 1 |
| Enter GRID of boundary condition in file "bc"- | 1 |
| Enter 1 to read boundary conditions from the terminal Enter 0 or n otherwise | 1 |
| For time step 1 enter number of new boundary conditions- | 4 |
| Enter BRANCH of new boundary condition- | 1 |
| Enter GRID of new boundary condition- | 2 |
| Temp Default= 0.0000000E+00 Value= | 21.5 |
| . | |
| . | |
| DO Default= 0.0000000E+00 Value= | 7.4 |
| . | |
| . | |
| Enter BRANCH of new boundary condition- | 1 |
| Enter GRID of new boundary condition- | 6 |
| Temp Default= 0.0000000E+00 Value= | 20.9 |
| . | |
| . | |
| DO Default= 0.0000000E+00 Value= | 7.4 |
| For time step 2 enter number of new boundary conditions- | 0 |
| . | |
| . | |
| For time step 48 enter number of new boundary conditions- | 0 |

Next, the initial number of parcels to be added in each subreach (IPPR) is requested. The accuracy of the model is highest if all parcels are of the same size; thus, for optimum accuracy, the model should begin with the same number of parcels in the system as the number of time steps required for a parcel to pass through the system. In this case, the approximate traveltime from the Route I-280 bridge to Fairburn is about 16 time steps (hours), so $16/6 = 3$ parcels per subreach should be entered. The program then requests the dispersion factor (DQQ) and initial concentration of all constituents for each subreach of each branch. All parcels in each subreach will be assigned the same initial concentration. The grid numbers where output is requested for the file "bltm.out" (3 and 7) are then input before moving on to the boundary values.

Boundary values for the upstream boundary are input from the file "bc" by entering the branch and grid number where the data are to be input. Because the boundary values for tributaries at grids 2, 3, 5, and 6 are constant, they are input from the terminal. After they are input for the first time step no boundary conditions are entered for any other time step. The model assumes all boundary conditions remain constant until changed by entering a new value.

Once the program BBLTM has been run with the input data shown in tables 2 (file "flow.in"), 4, 8 (file "bc"), and 9, it contains all the information except for the boundary conditions at grid 4, Utoy Creek, which are variable with time. The boundary values for Utoy Creek are shown in table 10.

The boundary conditions for Utoy Creek can be added to the file "bltm.in" by putting the data in table 10 to a file called "bc," copying the file "bltm.in" to a file called "old," and executing the program BBLTM again. When it is executed this time, however, the option to edit existing file is selected, and the data in file "bc" are entered for branch 1, grid 4. Boundary conditions are not entered from the terminal this time. Once this has been accomplished, the file "bltm.in" should be established as shown in table 11.

With the files "bltm.in" and "bltm.flw" established, the final step before QBLTM can be run is to establish the third input file "qual2e.in" (fig. 1).

The subroutine QUAL2E requires input of at least 28 different coefficients, 11 of which can be different in each subreach in each branch. It also requires values of equilibrium temperature, wind speed, and solar radiation at each time step. These data are read from a file called "*qual2e.in*" (fig. 1). The program BQUAL2E is designed to assist in creating the file "qual2e.in." Before this program is run, two things need to be done. First, the user should have some idea of the value of the reaction coefficients needed in the model. Default values are supplied in the program BQUAL2E, but there is no guarantee that these are applicable to the river reach in question. Second, a list or file "bc" of values for equilibrium temperature, wind speed, and solar radiation that have been averaged over each time step needs to be available.

Reports are available to help in estimating the reaction coefficients applicable to various rivers (Brown and Barnwell, 1987; Schnoor and others, 1987; Zison and others, 1978).

Table 10. Boundary conditions at Utoy Creek starting at hour 18.5 on May 31, 1977.

| Time | Temp | Algae | ON | NH3 | NO2 | NO | OP | PO4 | CBOD | DO |
|-------|-------|-------|------|------|------|------|------|------|-------|------|
| 18.50 | 21.81 | 0.00 | 1.20 | 7.62 | 0.01 | 0.21 | 0.48 | 1.71 | 18.10 | 5.31 |
| 19.50 | 21.81 | 0.00 | 1.20 | 7.73 | 0.01 | 0.21 | 0.46 | 1.80 | 17.27 | 5.29 |
| 20.50 | 21.84 | 0.00 | 1.20 | 7.61 | 0.01 | 0.21 | 0.43 | 1.97 | 18.16 | 5.26 |
| 21.50 | 21.86 | 0.00 | 1.20 | 7.48 | 0.02 | 0.21 | 0.39 | 2.14 | 19.06 | 5.24 |
| 22.50 | 21.89 | 0.00 | 1.20 | 7.36 | 0.02 | 0.21 | 0.36 | 2.31 | 19.96 | 5.21 |
| 23.50 | 21.87 | 0.00 | 1.24 | 7.16 | 0.02 | 0.21 | 0.36 | 2.35 | 20.85 | 5.19 |
| 24.50 | 21.81 | 0.00 | 1.32 | 6.88 | 0.02 | 0.21 | 0.41 | 2.25 | 21.50 | 5.17 |
| 25.50 | 21.75 | 0.00 | 1.40 | 6.60 | 0.01 | 0.22 | 0.46 | 2.15 | 21.90 | 5.15 |
| 26.50 | 21.69 | 0.00 | 1.48 | 6.32 | 0.01 | 0.22 | 0.51 | 2.05 | 22.30 | 5.13 |
| 27.50 | 21.63 | 0.00 | 1.56 | 6.04 | 0.01 | 0.22 | 0.56 | 1.95 | 22.70 | 5.11 |
| 28.50 | 21.63 | 0.00 | 1.60 | 5.84 | 0.01 | 0.22 | 0.51 | 1.85 | 23.10 | 5.13 |
| 29.50 | 21.67 | 0.00 | 1.60 | 5.71 | 0.01 | 0.22 | 0.38 | 1.75 | 22.99 | 5.18 |
| 30.50 | 21.73 | 0.00 | 1.60 | 5.59 | 0.01 | 0.21 | 0.25 | 1.65 | 22.36 | 5.22 |
| 31.50 | 21.77 | 0.00 | 1.60 | 5.46 | 0.01 | 0.21 | 0.12 | 1.55 | 21.74 | 5.28 |
| 32.50 | 21.85 | 0.00 | 1.51 | 5.50 | 0.01 | 0.21 | 0.06 | 1.40 | 21.11 | 5.31 |
| 33.50 | 21.95 | 0.00 | 1.33 | 5.70 | 0.01 | 0.21 | 0.08 | 1.20 | 19.79 | 5.33 |
| 34.50 | 22.05 | 0.00 | 1.15 | 5.90 | 0.01 | 0.21 | 0.09 | 1.00 | 17.77 | 5.35 |
| 35.50 | 22.15 | 0.00 | 0.97 | 6.10 | 0.02 | 0.21 | 0.11 | 0.80 | 15.75 | 5.37 |
| 36.50 | 22.25 | 0.00 | 0.79 | 6.30 | 0.02 | 0.21 | 0.13 | 0.60 | 13.73 | 5.39 |
| 37.50 | 22.30 | 0.00 | 0.70 | 6.58 | 0.02 | 0.21 | 0.14 | 0.47 | 11.71 | 5.41 |
| 38.50 | 22.30 | 0.00 | 0.70 | 6.93 | 0.02 | 0.21 | 0.16 | 0.43 | 10.40 | 5.44 |
| 39.50 | 22.30 | 0.00 | 0.70 | 7.28 | 0.02 | 0.21 | 0.17 | 0.38 | 9.80 | 5.46 |
| 40.50 | 22.30 | 0.00 | 0.70 | 7.63 | 0.02 | 0.21 | 0.18 | 0.33 | 9.20 | 5.49 |
| 41.50 | 22.29 | 0.00 | 0.88 | 7.80 | 0.02 | 0.21 | 0.19 | 0.54 | 8.60 | 5.50 |
| 42.50 | 22.26 | 0.00 | 1.22 | 7.80 | 0.02 | 0.21 | 0.22 | 1.01 | 10.11 | 5.50 |
| 43.50 | 22.24 | 0.00 | 1.57 | 7.80 | 0.02 | 0.22 | 0.25 | 1.49 | 13.74 | 5.50 |
| 44.50 | 22.21 | 0.00 | 1.92 | 7.80 | 0.02 | 0.22 | 0.28 | 1.96 | 17.36 | 5.50 |
| 45.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 20.99 | 5.50 |
| 46.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 47.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 48.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 49.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 50.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 51.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 52.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 53.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 54.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 55.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 56.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 57.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 58.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 59.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 60.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 61.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 62.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 63.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 64.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |
| 65.50 | 22.20 | 0.00 | 2.10 | 7.80 | 0.02 | 0.22 | 0.29 | 2.20 | 22.80 | 5.50 |

Table 11. Input file "bltm.in" of the QBLTM for the Chattahoochee River example.

```

Chattahoochee example problem
HEADER 1 1 0 48 10 18 1 1 0 1
HEADER 2 1.00 0.00
LABEL 1 Temp 1
LABEL 2 Alga 2
LABEL 3 ON 3
LABEL 4 NH3 4
LABEL 5 NO2 5
LABEL 6 NO3 5
LABEL 7 OP 7
LABEL 8 PO4 7
LABEL 9 CBOD 9
LABEL 10 DO 10
Branch 1 7 1 2 3
Grid 1 4.200 0 0.060 30.60 0.00 1.10 2.47 0.04 0.40 0.23
0.44 16.50 8.70
Grid 2 7.840 0 0.060 29.90 0.00 0.60 1.60 0.01 0.46 0.17
0.17 17.00 7.40
Grid 3 8.690 1 0.060 29.30 0.00 0.60 1.60 0.01 0.60 0.17
0.17 17.00 7.90
Grid 4 11.400 0 0.060 27.60 0.00 0.83 1.30 0.02 0.61 0.16
0.35 16.70 6.9
Grid 5 14.390 0 0.060 26.10 0.00 0.63 1.10 0.05 0.56 0.12
0.35 17.0 6.80
Grid 6 19.430 0 0.060 26.20 0.00 0.58 1.00 0.05 0.65 0.10
0.38 17.2 6.80
Grid 7 21.180 1
Time 1 6
B 1 G 1 29.62 0.00 0.93 2.50 0.04 0.32 0.22 0.55 17.33 8.68
B 1 G 2 21.50 0.00 1.70 1.50 0.02 0.50 0.40 0.70 28.70 7.40
B 1 G 3 20.80 0.00 8.30 13.00 0.08 0.04 2.90 6.00 86.30 0.60
B 1 G 4 21.81 0.00 1.20 7.62 0.01 0.21 0.48 1.71 18.10 5.31
B 1 G 5 21.70 0.00 0.47 0.05 0.01 0.28 0.04 0.00 5.10 7.70
B 1 G 6 20.90 0.00 0.48 1.20 0.03 0.80 0.05 1.10 5.50 7.40
Time 2 2
B 1 G 1 29.86 0.00 0.78 2.50 0.04 0.35 0.16 0.48 16.48 8.63
B 1 G 4 21.81 0.00 1.20 7.73 0.01 0.21 0.46 1.80 17.27 5.29
.
.
Time 47 1
B 1 G 1 29.25 0.00 0.65 1.50 0.04 0.39 0.09 0.15 11.00 7.90
Time 48 1
B 1 G 1 29.13 0.00 0.67 1.50 0.04 0.39 0.09 0.15 11.00 7.90

```

The program EQUULTMP is designed to estimate the needed equilibrium temperature values and wind speed by using readily available data from the National Weather Service. Table 12 contains a summary of the needed information obtained from the Local Climatological Data (monthly summary) for Atlanta, Ga., for 1977.

Table 12. Local climatological data for Hartsfield Atlanta International Airport, latitude 33 deg 39 min north, longitude 84 deg 26 min west, ground elev 1010 ft.

| Month | Day | Hour | Cloud cover | Air Temp °F | Dew Point °F | Wind mi/hr | |
|-------|-----|------|-------------|-------------|--------------|------------|---|
| May | 30 | 13 | | 85 | | | |
| | | 16 | | 82 | | | |
| | | 19 | | 78 | | | |
| | | 22 | | 72 | | | |
| | 31 | 1 | | | 71 | | |
| | | 4 | | | 68 | | |
| | | 7 | | | 67 | | |
| | | 10 | | | 76 | | |
| | | 13 | 0.8 | | 83 | 65 | 5 |
| | | 16 | | | 84 | | |
| June | 1 | 19 | | 75 | | | |
| | | 22 | | 71 | | | |
| | | 1 | | 67 | | | |
| | | 4 | | 67 | | | |
| | | 7 | | 69 | | | |
| | | 10 | | 78 | | | |
| | | 13 | 0.6 | | 85 | 60 | 8 |
| | 2 | 16 | | | 85 | | |
| | | 19 | | | 82 | | |
| | | 22 | | | 73 | | |
| | | 1 | | | 68 | | |
| | | 4 | | | 61 | | |
| | | 7 | | | 66 | | |
| | | 10 | | | 78 | | |
| 3 | 13 | 0.6 | | 77 | 54 | 9 | |
| | 16 | | | 81 | | | |
| | 19 | | | 79 | | | |
| | 22 | | | 68 | | | |
| | 1 | | | 66 | | | |
| | 3 | 4 | | 63 | | | |
| | | 7 | | 69 | | | |

Executing the program EQUULTMP with the default value of thermal air mass and selecting all other data from table 12, the output file "out" contains 3 full days of equilibrium temperature values. The output of the program EQUULTMP for the first full day is shown in table 13. Notice that the file contains the standard two lines of text information at the beginning. The first column represents the time of the computed values, which are centered on the time step; the second column is the estimated equilibrium temperature, in degrees Celsius; the third column is the wind speed in meter per second; and the fourth column, which is not used by the model, is the interpolated air temperature, in degrees Celsius. Rather than drawing a smooth curve through the points and interpolating the times of the minimum temperatures, it was assumed for this example that the maximum/minimum temperatures occurred on the hour shown in table 12. The format in table 13 is acceptable for input to the programs MRG or BQUAL2E. The name of the file "out" should be changed to "old.bc" so that it can be read by the program MRG and so that it will not be overwritten by later programs.

Table 13. Output of program EQUULTMP for May 31, 1977.

| Example problem for Atlanta Georgia | | | |
|-------------------------------------|---------|------|-------|
| Time | Equil C | M/s | Air T |
| 0.50 | 17.06 | 2.23 | 72.20 |
| 1.50 | 16.81 | 2.23 | 70.84 |
| 2.50 | 16.80 | 2.23 | 69.64 |
| 3.50 | 17.01 | 2.23 | 68.63 |
| 4.50 | 17.45 | 2.23 | 67.84 |
| 5.50 | 18.11 | 2.23 | 67.31 |
| 6.50 | 18.96 | 2.23 | 67.03 |
| 7.50 | 21.42 | 2.23 | 67.13 |
| 8.50 | 25.57 | 2.23 | 68.14 |
| 9.50 | 29.55 | 2.23 | 70.04 |
| 10.50 | 32.88 | 2.23 | 72.59 |
| 11.50 | 35.16 | 2.23 | 75.50 |
| 12.50 | 36.11 | 2.23 | 78.41 |
| 13.50 | 35.62 | 2.23 | 80.96 |
| 14.50 | 33.75 | 2.23 | 82.86 |
| 15.50 | 30.73 | 2.23 | 83.87 |
| 16.50 | 27.77 | 2.23 | 83.93 |
| 17.50 | 25.38 | 2.23 | 83.35 |
| 18.50 | 22.90 | 2.23 | 82.24 |
| 19.50 | 20.50 | 2.23 | 80.67 |
| 20.50 | 18.36 | 2.23 | 78.75 |
| 21.50 | 16.61 | 2.23 | 76.61 |
| 22.50 | 15.38 | 2.23 | 74.39 |
| 23.50 | 14.75 | 2.23 | 72.25 |

The program SOLAR can be used to estimate the solar radiation for each time step based on information available in table 12. The model starts on May 31, which is Julian day 151. Because Atlanta is in the eastern time zone and daylight saving time was in effect, the local time meridian is 60 degrees. A list of the output from the program SOLAR for May 31, 1977, is shown in table 14. These results are based on the data in table 12 and default values of all coefficients in the program. The output includes the two standard lines of text at the beginning plus a column of times and three columns of computed radiation values. The time of the estimated values is centered in the time step. The first column of computed values is the incoming solar radiation, the second column is the solar radiation that would have reached the surface under clear sky conditions, and the third column is the solar radiation at the top of the atmosphere. All radiation values are in Langley/min. Only the first column of computed values is used by the model. Notice that the largest clear-sky solar radiation (solar noon) occurs at 13.5 hours because Atlanta is near the western edge of the time zone and daylight saving time is in effect.

Table 14. Output of program SOLAR for May 31, 1977.

| Solar radiation for Atlanta | | | |
|-----------------------------|------|-------|-------|
| Time | Lang | Clear | Extra |
| 0.50 | 0.00 | 0.00 | 0.00 |
| 1.50 | 0.00 | 0.00 | 0.00 |
| 2.50 | 0.00 | 0.00 | 0.00 |
| 3.50 | 0.00 | 0.00 | 0.00 |
| 4.50 | 0.00 | 0.00 | 0.00 |
| 5.50 | 0.00 | 0.00 | 0.00 |
| 6.50 | 0.01 | 0.02 | 0.03 |
| 7.50 | 0.14 | 0.26 | 0.34 |
| 8.50 | 0.32 | 0.59 | 0.72 |
| 9.50 | 0.49 | 0.93 | 1.08 |
| 10.50 | 0.66 | 1.18 | 1.39 |
| 11.50 | 0.77 | 1.41 | 1.63 |
| 12.50 | 0.85 | 1.55 | 1.79 |
| 13.50 | 0.88 | 1.61 | 1.85 |
| 14.50 | 0.86 | 1.58 | 1.82 |
| 15.50 | 0.79 | 1.45 | 1.68 |
| 16.50 | 0.68 | 1.25 | 1.46 |
| 17.50 | 0.53 | 0.98 | 1.16 |
| 18.50 | 0.37 | 0.67 | 0.82 |
| 19.50 | 0.19 | 0.34 | 0.44 |
| 20.50 | 0.03 | 0.05 | 0.08 |
| 21.50 | 0.00 | 0.00 | 0.00 |
| 22.50 | 0.00 | 0.00 | 0.00 |
| 23.50 | 0.00 | 0.00 | 0.00 |

This completes the description of level 1 programs (fig. 1) for generating basic meteorologic data needed to drive the model. However, the equilibrium temperature and wind speed are in one file "old.bc" and the solar radiation is in another file "out." These data need to be in a single file "bc" before they can be used by the program BQUAL2E (fig. 1). The program MRG can be used to merge the first column of data, after the time column, from the file "in" to any column, after the time column, in the file "old.bc." To accomplish this, the file "out" must be copied to the file "in," and the program MRG must be executed. The program MRG asks for the number of columns of data in the file "old.bc" (three in this case—equilibrium temperature, wind speed, and air temperature) and for the column number to be changed. Again, this is column three because the air temperature values must be replaced with the solar radiation values from file "in." Table 15 contains the first 24 values of the merged data written in file "bc." Notice that the last column in file "old.bc" has been replaced with the solar radiation values, but the heading has not changed. It is suggested that this column heading be changed manually to indicate the new data. Both programs, SOLAR and EQUULTMP, compute values for the entire day even though the model is to start at 1800 hours. All data before 18.5 hours should be deleted from the file because the program BQUAL2E does not read the time column; it simply assumes that the first line of data in the file "bc" represents the first time step in the model.

Table 15. Output of program MRG for May 31, 1977.

| Example data for Atlanta Georgia | | | |
|----------------------------------|-------|------|-------|
| Time | Equ C | M/s | Air T |
| 0.50 | 17.06 | 2.23 | 0.00 |
| 1.50 | 16.81 | 2.23 | 0.00 |
| 2.50 | 16.80 | 2.23 | 0.00 |
| 3.50 | 17.01 | 2.23 | 0.00 |
| 4.50 | 17.45 | 2.23 | 0.00 |
| 5.50 | 18.11 | 2.23 | 0.00 |
| 6.50 | 18.96 | 2.23 | 0.01 |
| 7.50 | 21.42 | 2.23 | 0.14 |
| 8.50 | 25.57 | 2.23 | 0.32 |
| 9.50 | 29.55 | 2.23 | 0.49 |
| 10.50 | 32.88 | 2.23 | 0.65 |
| 11.50 | 35.16 | 2.23 | 0.77 |
| 12.50 | 36.11 | 2.23 | 0.85 |
| 13.50 | 35.62 | 2.23 | 0.98 |
| 14.50 | 33.75 | 2.23 | 0.86 |
| 15.50 | 30.73 | 2.23 | 0.79 |
| 16.50 | 27.77 | 2.23 | 0.68 |
| 17.50 | 25.38 | 2.23 | 0.53 |
| 18.50 | 22.90 | 2.23 | 0.37 |
| 19.50 | 20.50 | 2.23 | 0.19 |
| 20.50 | 18.36 | 2.23 | 0.03 |
| 21.50 | 16.61 | 2.23 | 0.00 |
| 22.50 | 15.38 | 2.23 | 0.00 |
| 23.50 | 14.75 | 2.23 | 0.00 |

With the file "bc" which contains the meteorological data needed for the model created, the program BQUAL2E can be run to create a file "qual2e.in," which is the last file needed by QBLTM. Table 16 contains the file generated by BQUAL2E when the limiting nutrient growth rate option and all defaults are assumed. Variables are identified by their Fortran names in the code. Coefficients that are variable with subreach are entered on two lines to keep the line length under 80 characters.

Table 16. Input file "qual2e.in" for QUAL2E subroutine of the QBLTM model.

```

Water quality of Chattahoochee
Wind function = A1 + B1 V [mm/(day kpa)], Wind speed V in m/s
                3.01  1.13
ALPH0 ALPH1 ALPH2 ALPH3 ALPH4 ALPH5 ALPH6 GROMAX IGRO RSPRT
 50.0  0.080  0.015  1.60  2.00  3.50  1.12  2.00  2  0.20
LFO CKL CKN CKP SHAD0 SHAD1 SHAD2 PN K2O
1  5.000 0.300 0.040 0.100 0.003 0.000 0.500 1
Br Gr ALGSET BET3 SIG4 BET1 SIG3 BET2 BET4
1 1  1.50  0.200 0.010 0.300 3.000 1.50 0.400
1 2  1.50  0.200 0.010 0.300 3.000 1.50 0.400
1 3  1.50  0.200 0.010 0.300 3.000 1.50 0.400
1 4  1.50  0.200 0.010 0.300 3.000 1.50 0.400
1 5  1.50  0.200 0.010 0.300 3.000 1.50 0.400
1 6  1.50  0.200 0.010 0.300 3.000 1.50 0.400
Br Gr SIG5 SIG2 CK1 CK3 CK4 CK2
1 1  0.200 1.000 0.340 0.240 20.000 2.200 0.00
1 2  0.200 1.000 0.340 0.240 20.000 2.200 0.00
1 3  0.200 1.000 0.340 0.240 20.000 2.200 0.00
1 4  0.200 1.000 0.340 0.240 20.000 2.200 0.00
1 5  0.200 1.000 0.340 0.240 20.000 2.200 0.00
1 6  0.200 1.000 0.340 0.240 20.000 2.200 0.00
Time  TE C  V, m/s  Solar cal/cm^2 min
18.5  22.90  2.23  0.370
19.5  20.50  2.23  0.190
.
.
.
16.5  26.04  4.02  0.930
17.5  23.50  4.02  0.730

```

With the three input files "bltm.in," "bltm.flw," and "qual2e.in" available, the program QBLTM can be run to predict the concentrations throughout the river reach during the 48-hour simulation period.

Table 17 contains a partial listing of the output, which is written to the file "bltm.out." The first part of the output contains input data to the model. Listing this input information allows the user to be sure the model inputs are as intended. Next, the section titled "INITIAL CONDITIONS" contains the initial concentrations and hydraulic conditions for each subreach. For example, at time zero the discharge at grid 2, located 7.84 miles downstream of the reference point, was 1,278 ft³/s, and the average cross-sectional area and channel top width for the subreach that extends from grid 2 to grid 3 were 865.63 ft² and 199.09 ft, respectively. Notice that the flow at grid 2 is 28 ft³/s larger than at grid 1 because the 28 ft³/s of tributary inflow at grid 2 is assumed to enter

just upstream of the grid point. The initial temperature of the water between grids 2 and 3 is 29.90°C. The dispersion factor in the subreach is 0.06.

Following the initial conditions, a listing of all assumed reaction coefficients is given in a self-explanatory format.

The final section contains the computed concentrations at selected locations for a specified time frequency. In addition to the computed concentrations, various information about the history of the water at the point is given. This information can help the user understand the effects of various assumptions on the computed results.

Table 17 contains the output at grid 3, South Cobb Creek, and grid 7, Fairburn, for day 2, hours 6 and 18.

Consider the output for Fairburn, grid 7, at 0600 hours on June 1, 1977 (day 2, hour 6). Because $K=18$, there are currently 17 water parcels upstream of the 1 located at Fairburn. The volume of the parcel (PV) located at Fairburn is equal to the volume of the parcel upstream of the grid (VU) because grid 7 is the last grid in the branch. Parcel 18 contains 1,030,000 ft³ of water. The time the parcel entered the branch (PH) is listed as -6; the minus is a code that indicates that the parcel was in the branch at time zero; and the 6 indicates that it was the sixth parcel, when counted from upstream. In other words, the water located at Fairburn at 0600 hours on June 1, 1977, had been located in the lower one-third of the subreach between grids 2 and 3 at 1800 hours on May 31, 1977 [recall that three parcels were entered for each subreach, table 9 (IPPR=3)]. The current concentrations of each constituent, which are then listed, indicate the water temperature at this time is 25.019°C and the dissolved-oxygen concentration is 5.578 mg/L. The next line, labeled "PTI", lists the concentrations the parcel contained when it entered the system. In this case, the parcel was already located in the branch at time zero, so PTI lists its initial concentration. The output lists the initial water temperature as 29.9°C, which corresponds to the value given in table 4. The PDF line indicates that the temperature in this parcel was reduced by 0.219°C as a result of longitudinal dispersion. The PTR line of output indicates that the water parcel was cooled by 1.036°C as a result of tributary inflow. Finally, the PDC line indicates that the water temperature of the parcel decreased by 3.626°C as a result of surface exchange with the atmosphere. The value of PDC is known to represent surface exchange because the value of LR was selected as 1, table 9. All processes that contributed to the change in the computed water temperature from the start of the model to the current time are tracked in the output, which can be verified as follows. The current temperature (25.019) should equal the initial temperature (29.900) plus all changes (29.900 - 0.219 - 1.036 - 3.626 = 25.019).

Next, consider the water located at grid 3 at 0600 hours on June 1. Because $K=5$, this is the fifth water parcel in the system indicating 4 full hours have passed since the particle entered at the Route I-280 bridge. The volume of this parcel is 4,630,000 ft³ (PV), and 2,290,000 ft³ (VU) are still upstream of the grid. Because 49.5 percent of the parcel has not passed the grid at 0600 hours, the traveltime from Route I-280 to grid 2 is 4.495 hours. Alternatively, the water entered the system at hour 26 (PH), actually between hours 25 and 26, so the traveltime can be roughly estimated as between $6 - 1 = 5$ and $6 - 2 = 4$ hours from the current time and the time the parcel entered the system. The other information is the same as that discussed for the water at Fairburn.

Table 17. Output of the BLTM model for the Chattahoochee River, Atlanta to Fairburn, Ga.

Chattahoochee example problem

The 1 Branch model has 0 Internal junctions.
 48 Time steps are run, each 1.00 Hours long.
 The model starts at 18.00 Hours past midnight.
 The grid output is given in "bltm.out" every 1 Time steps.
 The parcel output is given in "parcel.out" every 1 Time steps.
 10 Constituents are routed and the Minimum Dispersive velocity is 0.000 ft/s.
 Flow conditions from DAFLOW used
 Input units are English (feet and river miles)

INITIAL CONDITIONS

| Grid | River Mile | Discharge cu ft/s | Area sq ft | Top Width feet | Trib. Flow | | Alga | ON | Initial Concentration | | | | | | | |
|--|---------------|-------------------|------------|----------------|------------|-------|------|------|-----------------------|------|------|------|------|-------|------|--|
| | | | | | cu ft/s | Temp | | | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO | |
| Branch 1 Extends from JUCT 1 to junction 2 | | | | | | | | | | | | | | | | |
| 1 | 4.20 | 1250.00 | 855.24 | 197.95 | 0.00 | 30.60 | 0.00 | 1.10 | 2.47 | 0.04 | 0.40 | 0.23 | 0.44 | 16.50 | 8.70 | |
| DQQ = | 5.9999999E-02 | | | | | | | | | | | | | | | |
| 2 | 7.84 | 1278.00 | 865.63 | 199.09 | 28.00 | 29.90 | 0.00 | 0.60 | 1.60 | 0.01 | 0.46 | 0.17 | 0.17 | 17.00 | 7.40 | |
| DQQ = | 5.9999999E-02 | | | | | | | | | | | | | | | |
| 3 | 8.69 | 1292.00 | 870.80 | 199.66 | 14.00 | 29.30 | 0.00 | 0.60 | 1.60 | 0.01 | 0.60 | 0.17 | 0.17 | 17.00 | 7.90 | |
| DQQ = | 5.9999999E-02 | | | | | | | | | | | | | | | |
| 4 | 11.40 | 1321.00 | 881.47 | 200.82 | 29.00 | 27.60 | 0.00 | 0.83 | 1.30 | 0.02 | 0.61 | 0.16 | 0.35 | 16.70 | 6.90 | |
| DQQ = | 5.9999999E-02 | | | | | | | | | | | | | | | |
| 5 | 14.39 | 1476.00 | 937.31 | 206.69 | 155.00 | 26.10 | 0.00 | 0.63 | 1.10 | 0.05 | 0.56 | 0.12 | 0.35 | 17.00 | 6.80 | |
| DQQ = | 5.9999999E-02 | | | | | | | | | | | | | | | |
| 6 | 19.43 | 1509.00 | 948.96 | 207.88 | 33.00 | 26.20 | 0.00 | 0.58 | 1.00 | 0.05 | 0.65 | 0.10 | 0.38 | 17.20 | 6.80 | |
| DQQ = | 5.9999999E-02 | | | | | | | | | | | | | | | |
| 7 | 21.18 | 1509.00 | | | | | | | | | | | | | | |

Water quality of Chattahoochee
 Wind function = 3.01+ 1.13V [mm/day KPA when V is in M/s].

Reaction Kinetics

Chlorophyll-A content, Algae ALPH0= 50.0 ug-Chl/mg-A
 Nitrogen content of algae ALPH1= 0.080 mg-N/mg-A
 Phosphorus content of algae ALPH2= 0.015 mg-P/mg-A
 DO produced/ algae growth ALPH3= 1.60 mg-O/mg-A
 DO used/ unit algae respired ALPH4= 2.00 mg-O/mg-A
 DO used/unit ammonia oxidized ALPH5= 3.50 mg-O/mg-N
 DO used/unit nitrite oxidized ALPH6= 1.12 mg-O/mg-N
 Maximum specific growth rate GROMAX= 2.00 per day

Table 17. Output of BLTM model for Chattahoochee River, Atlanta to Fairburn, Ga. —(continued)

Respiration rate for algae RSPRT= 0.20 per day

Nutrient limiting growth

Light intensity @ 50% of grwth CKL= 5.000 cal/cm^2 min

Nitrogen half-saturation const CKN= 0.300 mg-N/L

Phos half-saturation constant CKP= 0.040 mg-P/L

Light extinction coef = 0.100 + 0.30E-02 Chl-A + 0.00E+00 Chl-A^2/3

Preference factor for ammonia nitrogen PN= 0.500

Use reaeration option K2O= 1

| Br | Gr | ALGSET | BET3 | SIG4 | BET1 | SIG3 | BET2 | BET4 |
|----|----|--------|-------|-------|-------|-------|------|-------|
| 1 | 1 | 1.50 | 0.200 | 0.010 | 0.300 | 3.000 | 1.50 | 0.400 |
| 1 | 2 | 1.50 | 0.200 | 0.010 | 0.300 | 3.000 | 1.50 | 0.400 |
| 1 | 3 | 1.50 | 0.200 | 0.010 | 0.300 | 3.000 | 1.50 | 0.400 |
| 1 | 4 | 1.50 | 0.200 | 0.010 | 0.300 | 3.000 | 1.50 | 0.400 |
| 1 | 5 | 1.50 | 0.200 | 0.010 | 0.300 | 3.000 | 1.50 | 0.400 |
| 1 | 6 | 1.50 | 0.200 | 0.010 | 0.300 | 3.000 | 1.50 | 0.400 |

| Br | Gr | SIG5 | SIG2 | CK1 | CK3 | CK4 | CK2 |
|----|----|-------|-------|-------|-------|--------|--------|
| 1 | 1 | 0.200 | 1.000 | 0.340 | 0.240 | 20.000 | 2.2000 |
| 1 | 2 | 0.200 | 1.000 | 0.340 | 0.240 | 20.000 | 2.2000 |
| 1 | 3 | 0.200 | 1.000 | 0.340 | 0.240 | 20.000 | 2.2000 |
| 1 | 4 | 0.200 | 1.000 | 0.340 | 0.240 | 20.000 | 2.2000 |
| 1 | 5 | 0.200 | 1.000 | 0.340 | 0.240 | 20.000 | 2.2000 |
| 1 | 6 | 0.200 | 1.000 | 0.340 | 0.240 | 20.000 | 2.2000 |

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| Day | 2 Hour | 6.0 | VU | PV | PH | Temp | Alga | ON | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO |
|------|--------|-------|-----------|-----------|-------|--------|------|--------|--------|--------|--------|--------|-------|--------|--------|
| Br 1 | Grid 3 | K= 5 | 0.229E+07 | 0.463E+07 | 26.00 | 25.460 | 0.00 | 1.059 | 1.982 | 0.136 | 0.383 | 0.206 | 0.557 | 13.414 | 6.889 |
| | | | | PTI | | 26.520 | 0.00 | 1.050 | 2.000 | 0.040 | 0.350 | 0.210 | 0.500 | 14.100 | 8.200 |
| | | | | PDF | | -0.014 | 0.00 | 0.002 | 0.008 | 0.000 | 0.002 | 0.002 | 0.003 | 0.201 | -0.022 |
| | | | | PTR | | -0.119 | 0.00 | 0.055 | 0.051 | -0.002 | 0.001 | 0.019 | 0.034 | 0.741 | -0.032 |
| | | | | PDC | | -0.927 | 0.00 | -0.047 | -0.128 | -0.030 | 0.000 | -0.025 | 0.000 | -1.627 | 0.270 |
| | | | | | | | | | | | | | | | |
| Br 1 | Grid 7 | K= 18 | 0.103E+07 | 0.103E+07 | -6.00 | 25.019 | 0.00 | 0.607 | 1.489 | 0.202 | 0.628 | 0.121 | 0.328 | 10.869 | 5.578 |
| | | | | PTI | | 29.900 | 0.00 | 0.600 | 1.600 | 0.010 | 0.460 | 0.170 | 0.170 | 17.000 | 7.400 |
| | | | | PDF | | -0.219 | 0.00 | 0.026 | 0.045 | 0.008 | 0.071 | -0.007 | 0.010 | -0.416 | 0.344 |
| | | | | PTR | | -1.036 | 0.00 | 0.073 | 0.068 | -0.019 | -0.033 | 0.020 | 0.098 | -0.413 | 0.141 |
| | | | | PDC | | -3.626 | 0.00 | -0.092 | -0.332 | -0.130 | 0.000 | -0.062 | 0.000 | -5.302 | 2.436 |

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Table 17. Output of BLTM model for Chattahoochee River, Atlanta to Fairburn, Ga. — (continued)

| Day | 2 Hour | 18.0 | VU | PV | PH | Temp | Alga | ON | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO | |
|------|--------|-------|-----------|-----------|-------|--------|--------|-------|--------|--------|--------|--------|--------|--------|--------|--------|
| Br 1 | Grid 3 | K= 5 | 0.229E+07 | 0.463E+07 | 38.00 | 28.188 | 0.00 | 1.605 | 1.629 | 0.125 | 0.421 | 0.397 | 0.333 | 14.113 | 6.540 | |
| | | | | | | PTI | 28.330 | 0.00 | 1.500 | 1.650 | 0.040 | 0.390 | 0.450 | 0.230 | 15.380 | 7.970 |
| | | | | | | PDF | -0.012 | 0.00 | 0.144 | -0.047 | 0.001 | -0.001 | -0.009 | 0.020 | -0.083 | 0.029 |
| | | | | | | PTR | -0.195 | 0.00 | 0.040 | 0.061 | -0.002 | 0.000 | 0.014 | 0.041 | 0.719 | -0.024 |
| | | | | | | PDC | 0.065 | 0.00 | -0.078 | -0.118 | -0.032 | 0.000 | -0.057 | 0.000 | -1.903 | 0.256 |
| Br 1 | Grid 7 | K= 17 | 0.221E+07 | 0.221E+07 | 26.00 | 26.704 | 0.00 | 0.876 | 1.675 | 0.259 | 0.582 | 0.132 | 0.600 | 9.104 | 5.549 | |
| | | | | | | PTI | 26.520 | 0.00 | 1.050 | 2.000 | 0.040 | 0.350 | 0.210 | 0.500 | 14.100 | 8.200 |
| | | | | | | PDF | -0.002 | 0.00 | -0.021 | 0.002 | 0.000 | 0.008 | 0.000 | -0.003 | 0.343 | -0.032 |
| | | | | | | PTR | -0.890 | 0.00 | 0.030 | -0.035 | -0.036 | -0.015 | 0.013 | 0.032 | 0.431 | 0.157 |
| | | | | | | PDC | 1.077 | 0.00 | -0.184 | -0.494 | -0.239 | 0.000 | -0.091 | 0.000 | -5.770 | 2.938 |

Finally, notice that the water at Fairburn on day 2, hour 18 (1800 hours on June 1), entered the branch during hour 26 (PH= 26) which indicates that this is the same water that was located at grid 2 at 0600 hours of the same morning. The effect of various processes on the concentrations that occur in the reach between grid 2 and Fairburn can be determined by comparing the changes that occur throughout the entire branch (given at grid 7) to those that occur in the subreach from grid 1 to grid 3 given at grid 3 for day 2, hour 6. For example, surface exchange had increased the water temperature by 1.077°C when averaged over the entire passage through the branch; but when averaged over the time required to move from Route I-280 to grid 3, it had decreased the water temperature by 0.927°C. Therefore, from 0200 hours until 0600 hours on June 1, the water cooled by 0.927°C; but during the day, from 0600 to 1800 hours, it warmed a total of $1.077 - (-0.927) = 2.004^\circ\text{C}$. In calibrating a model, it is very helpful to concentrate attention on water parcels that pass two or more points at times when observations are available. Construction of a rough figure as illustrated in figure 5 is often helpful in determining where to concentrate one's effort. It is readily seen that the four data points that are solid (along parcel, PH = 3) are more useful for evaluating the accuracy of the model in simulating changes than the other points. Unless two or more data points occur near a single parcel track, little information about the accuracy of the model can be gained.

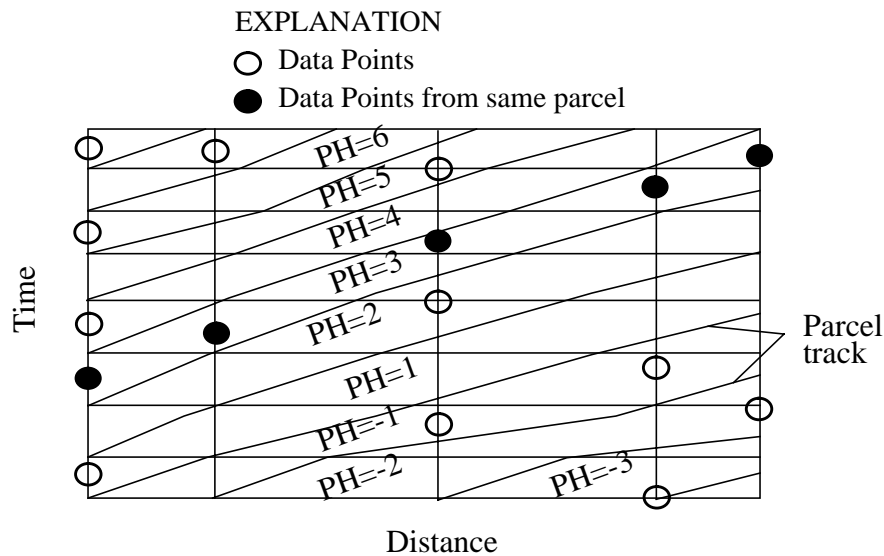


Figure 5. Water parcel tracks in the space-time domain relative to the location of data points.

For a single run, the effect of only one chemical reaction can be tabulated by using PDC. The specific reaction to be tabulated is specified by use of the variable LR. If more than one reaction is to be evaluated, then the model can be run multiple times with different values assigned to LR. It can be seen from figure 4, for example, that four processes affect the kinetics of ammonia—decay of organic nitrogen to ammonia (BET3), uptake by algae (GRO ALPH1 F1), decay of ammonia to nitrite (CORDO BET1), and benthic production (SIG3). Zero-order rate terms, such as the benthic production term (SIG3) cannot be tabulated by use of PDC, but the other three terms can. The model was run three times with the various values assigned to LR. Table 18 contains the output at Fairburn for day 2, hour 18, along with the assigned values of LR.

Table 18. Output at Fairburn, Ga., on day 2, hour 18 for various values of LR

| Day 2 Hour 18.0 | VU | PV | PH | Temp | Alga | ON | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO |
|-------------------|-----------|-----------|-------|--------|------|--------|--------|--------|--------|--------|--------|--------|--------|
| Br 1 Grid 7 K= 17 | 0.221E+07 | 0.221E+07 | 26.00 | 26.704 | 0.0 | 0.876 | 1.675 | 0.259 | 0.582 | 0.132 | 0.600 | 9.104 | 5.549 |
| | | | PTI | 26.520 | 0.0 | 1.050 | 2.000 | 0.040 | 0.350 | 0.210 | 0.500 | 14.100 | 8.200 |
| | | | PDF | -0.002 | 0.0 | -0.021 | 0.002 | 0.000 | 0.008 | 0.000 | -0.003 | 0.343 | -0.032 |
| | | | PTR | -0.890 | 0.0 | 0.030 | -0.035 | -0.036 | -0.015 | 0.013 | 0.032 | 0.431 | 0.157 |
| | | | PDC | 1.077 | 0.0 | 0.000 | 0.000 | 0.000 | 0.000 | -0.091 | 0.063 | -5.770 | -3.568 |
| | | | LR = | 1 | 2 | 2 | 2 | 2 | 2 | 7 | 7 | 9 | 9 |
| | | | | | | | | | | | | | |
| Day 2 Hour 18.0 | VU | PV | PH | Temp | Alga | ON | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO |
| Br 1 Grid 7 K= 17 | 0.221E+07 | 0.221E+07 | 26.00 | 26.704 | 0.0 | 0.876 | 1.676 | 0.259 | 0.582 | 0.132 | 0.600 | 9.109 | 5.553 |
| | | | PTI | 26.520 | 0.0 | 1.050 | 2.000 | 0.040 | 0.350 | 0.210 | 0.500 | 14.100 | 8.200 |
| | | | PDF | -0.002 | 0.0 | -0.021 | 0.002 | 0.000 | 0.008 | 0.000 | -0.003 | 0.343 | -0.032 |
| | | | PTR | -0.890 | 0.0 | 0.030 | -0.035 | -0.036 | -0.015 | 0.013 | 0.032 | 0.431 | 0.157 |
| | | | PDC | 1.077 | 0.0 | -0.184 | 0.176 | -0.239 | 0.239 | 0.000 | 0.000 | -5.770 | -1.728 |
| | | | LR = | 1 | 2 | 3 | 3 | 5 | 5 | 2 | 8 | 9 | 4 |
| | | | | | | | | | | | | | |
| Day 2 Hour 18.0 | VU | PV | PH | Temp | Alga | ON | NH3 | NO2 | NO3 | OP | PO4 | CBOD | DO |
| Br 1 Grid 7 K= 17 | 0.221E+07 | 0.221E+07 | 26.00 | 26.704 | 0.0 | 0.876 | 1.676 | 0.259 | 0.582 | 0.132 | 0.600 | 9.109 | 5.553 |
| | | | PTI | 26.520 | 0.0 | 1.050 | 2.000 | 0.040 | 0.350 | 0.210 | 0.500 | 14.100 | 8.200 |
| | | | PDF | -0.002 | 0.0 | -0.021 | 0.002 | 0.000 | 0.008 | 0.000 | -0.003 | 0.343 | -0.032 |
| | | | PTR | -0.890 | 0.0 | 0.030 | -0.035 | -0.036 | -0.015 | 0.013 | 0.032 | 0.431 | 0.157 |
| | | | PDC | 1.077 | 0.0 | -0.184 | -0.494 | 0.494 | 0.000 | 0.000 | 0.000 | -5.770 | -0.268 |
| | | | LR = | 1 | 2 | 3 | 4 | 4 | 6 | 2 | 8 | 9 | 5 |

To illustrate the use of the PDC term consider the mass balance for ammonia of the water parcel located at Fairburn on day 2, hour 18.0. The concentration of the water as it passed the Route I-280 bridge was 2.000 mg/L. The water arrived at Fairburn a little more than 17 hours later with a computed concentration of 1.675, which is, of course, the same for any values of LR. Longitudinal dispersion increased its concentration by 0.002, and tributary inflow decreased its concentration by 0.035. From the first entry in table 18, with LR = 2, algae uptake was zero because the concentration of algae was assumed to be zero throughout. From the second entry, with LR = 3, 0.176 mg/L of ammonia was produced from organic nitrogen. Likewise, from the third entry, LR = 4, 0.494 mg/L was transformed into nitrite. Summing up the mass balance changes listed above, the computed concentration is $2.000 + 0.002 - 0.035 - 0.000 + 0.176 - 0.494 = 1.649$ mg/L. Because the actual computed concentration is 1.675, it can be inferred that the benthic source term (SIG3) has contributed 0.026 mg/L to the concentration of this water parcel. A similar mass balance could be performed for any of the constituents. It is very instructive to compare the magnitudes of the terms that contribute to the change in concentration of a water parcel with the errors in the computed concentrations. Figure 6 contains a plot of the computed and observed concentrations at Fairburn, which can be produced by use of the program CTPLT. As can be seen from the figure, the computed values at this time are about 0.2 mg/L larger than the observed values. This error can be compared with the magnitude of each of the mass balance terms before deciding which processes are most likely in error.

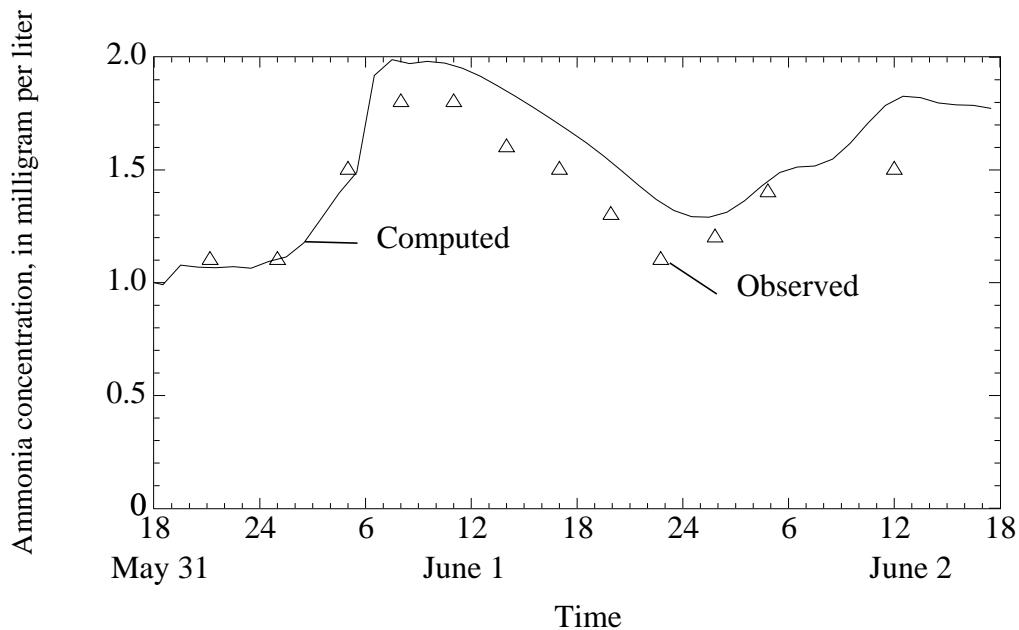


Figure 6. Computed and observed concentration of ammonia at Fairburn, Ga.

SUMMARY

The Branched Lagrangian Transport Model (BLTM) has received wide use within the U.S. Geological Survey over the past 10 years. This report documents the enhancements and modifications that have been made to this modeling system since it was first introduced. The programs in the modeling system are arranged into five levels —programs to generate time-series of meteorological data (EQUULTMP, SOLAR), programs to process time-series data (INTRP, MRG), programs to build input files for transport model (BBLTM, BQUAL2E), the model with defined reaction kinetics (BLTM, QUAL2E), and post processor programs (CTPLT, CXPLT). The modeling system was illustrated by simulating 10 water-quality constituents in 17-mile reach of the Chattahoochee River below Atlanta, Georgia.

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