Dynamic Toxics

Waste Load Allocation Model

(DYNTOX)

USER'S MANUAL

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PREFACE

This report represents a Users Manual to explain how to use the DYNTOX model. This computer model was developed by Limno-Tech, Inc. under direction from the U.S. Environmental Protection Agency Monitoring and Data Support Division. It is designed for use in waste load allocation of toxic substances. It uses three simulation techniques to calculate the frequency and severity of instream toxicity at different effluent discharge levels. The report is contained in two volumes, consisting of the User's Manual and a separately bound appendix. The User's Manual describes the theory behind each technique, their use in DYNTOX, and briefly discusses how to use DYNTOX when performing waste load allocations. The appendix provides two illustrative examples.

This report is not intended to be a discussion of the theoretical characteristics and practical nuances of the three techniques. Some introductory remarks are provided in these regards, but the primary objective of this report is to provide use instructions for the DYNTOX programs.

This project required the combined efforts of many individuals and organizations. These are highlighted below:

Funding support was provided by the U.S. Environmental Protection Agency Monitoring and Data Support Division (Contract #68-03-3131). Dr. Elizabeth Southerland was project officer and provided invaluable insights and direction to the project. Messrs. Tim Stuart and Mark Morris of EPA also provided valuable administrative direction. Jack Kittle of Anderson-Nichols is thanked for his assistance in supplying updated versions of the ANNIE program. Dr. Dominic DiToro, Manhattan College is thanked for his contribution to the log normal analysis aspects of the project. Drs. Paul Rodgers and Raymond Canale of Limno-Tech, Inc. are thanked for their conceptual ideas. Tad Slawecki and Dr. Derek Wong, also of Limno-Tech, Inc. are thanked for their program contributions.

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I. OVERVIEW

Environmental contamination by toxic substances can pose risks to public and ecological health. Regulatory agencies are now establishing regulations and procedures for determining allowable discharge limits to minimize those risks. Unfortunately, technology to define risks and quantify allowable discharge limits is new or not widely used or understood. This document serves to provide instructions on the use of modeling techniques for calculating allowable loading limits and the associated risks. These techniques are incorporated in the DYNTOX portion of the ANNIE interactive program.

Background

At present, most States which have regulations for setting allowable discharge limits for toxic pollutants use steady state models to assess exposure and calculate waste load allocations. These models are used to calculate the allowable effluent load that just meets the chronic toxicity water quality standard at a critical low flow. These analyses typically do not consider issues of frequency and duration. They generally consist only of a simple dilution equation; do not include instream processes; and only examine a single environmental condition for a single discharge at a single design specification.

In contrast, the extent of biological impairment from toxic discharges depends on the duration of exposure above certain levels as well as the number of times (frequency) these violations occur. Water quality criteria now specify both duration and frequency of compliance. The duration and frequency of violations depend on the daily variation in receiving water and effluent flow, combined with daily variation in effluent toxicity. Therefore dynamic models must be used to calculate the frequency distribution of instream concentrations for any given duration. The current durations of interest are four days for chronic toxicity and one hour for acute toxicity. The one hour duration period generally is approximated as a one day period because hourly data are generally not available.

Modeling techniques are available that incorporate the effects of both variable flow and effluent to calculate the frequency and duration of exposure at different concentration levels. These more thorough methods simulate the entire distribution of receiving water concentrations (expressed in a probability distribution) rather than a single "worst case" based on critical conditions. This allows each alternative control strategy to be evaluated in terms of the total risk of toxic concentration. The data used to define criteria for toxic levels of substances incorporate the concepts of duration and risk. It is only appropriate that the procedures used to regulate these substances also incorporate these concepts.

Concepts

Ideally, it would be desirable to assess the impacts of toxic discharges on receiving water quality over the entire range of historical and future conditions. These conditions would then be analyzed to define frequency and duration of exposure above specified limits. Unfortunately, on a practical basis this approach is impossible. However, three procedures are readily available which estimate this range of conditions. These are:

1. Continuous Simulation
2. Monte Carlo Simulation
3. Log Normal Analysis

All three are included in the DYNTOX program.

Continuous Simulation uses the most direct approach. A mathematical model is used to simulate a specified period of recorded history. This approach uses a historical record of river flow and upstream conditions combined with a historical or projected record of discharge flow and toxicity. Results from this simulation are then analyzed for frequency and duration of toxicity which are assumed to statistically describe the entire record. The procedure requires an extended period of record but is simple to execute and understand.

The Monte Carlo simulation technique is less direct but also involves a simple approach. It uses a model as Continuous Simulation, but inputs are not determined on a continuous basis. Inputs such as river flows, upstream conditions, effluent flow and effluent toxicity are each defined statistically by a distribution of historical or potential conditions. The Monte Carlo model then repetitively selects sets of model inputs randomly from among these statistical distributions. Statistical theory dictates that the distribution of results from numerous repetitive simulations will characterize the actual distribution of potential outcomes. This distribution can then be used to define frequency and duration of toxics concentrations. This technique requires either a good statistical characterization for model inputs or reasonable assumptions.

The Log Normal analysis procedure is computationally less extensive than the previous two simulation techniques but involves more complex theory and certain restrictions. This procedure assumes all input parameters follow a log normal statistical distribution. Statistical theory dictates that under these conditions for a simple dilution model with one discharge, the projected outcomes can be numerically determined. The procedure incorporates the distributions into the model through numerical integration and thereby defines the distribution of downstream water quality. This distribution can then be used to define the frequency and duration of different river concentrations. The procedure requires a proper log normal characterization for all model inputs.

The DYNTOX programs are at this time designed only for use in rivers and streams. Kinetic interactions are restricted to first order losses. Monte Carlo and Continuous Simulation are amenable to more sophisticated situations which were not included in this study. DYNTOX can be used to set up inputs for models of lakes and estuaries or for river models with more complex fate processes. At present DYNTOX does not include models to address these more complex situations.

Organization of Manual

The first chapter (after the overview) of this report describes those aspects common to all three simulation techniques. This includes general operation of the ANNIE program, how to access the three probabilistic models in DYNTOX, the required input data, and step by step procedures. The next three chapters discuss the theory behind Continuous Simulation, Monte Carlo simulation, and Log Normal. The final section includes a brief discussion on how to select the most suited technique for an individual wasteload allocation and qualitatively how to assess the reliability of the results.

Illustrative examples demonstrating the use of each of the three DYNTOX techniques are bound separately as an appendix to this report. This appendix also contains information on mainframe and microcomputer installation of DYNTOX.

II. COMMON REQUIREMENTS

The three analytical techniques contained in DYNTOX, although conceptually quite different, have several common requirements. The first common requirement is that the DYNTOX programs can only be accessed through the U.S. Geological Survey model pre-processor program ANNIE. This requirement was brought about to maintain consistency and continuity with the use of ANNIE as a preprocessor for large mainframe computer models. For future microcomputer adaptation of DYNTOX, the requirement of ANNIE-only access may be discontinued.

All three analytical techniques in DYNTOX also require the same three general types of input data:

1) Upstream data...used to describe flow and concentration in the river upstream of the discharge(s).

2) System data...used to describe such processes as `nstream decay, time of travel between outfalls, etc.

3) Effluent data...used to describe the flow and concentration of each discharge.

Upstream boundary flow and concentration data can be obtained through DYNTOX from STORET. In cases where STORET data are not available, the user may enter data directly from the terminal. System data must be determined by the user prior to performing any simulations. Effluent data must be supplied by the user and may either be read from a computer file or entered directly from the terminal.

This chapter describes the requirements common to all three techniques: how to access the model and how to obtain the three types of common required data in the appropriate format. Input format and inputs specific to a given technique will be discussed later in their respective chapters.

Model Access

Presently, DYNTOX is accessed through the computer program ANNIE. The ANNIE program was originally designed and supported by the U.S. Geological Survey in cooperation with the U.S. Environmental Protection Agency to help users interactively create, check and update inputs to models and perform the actual model simulation. Limno-Tech, Inc. has added the capability of probabilistic simulation. Presently, the only way DYNTOX can be accessed is through ANNIE. This section briefly describes the ANNIE program and how it is used to access DYNTOX.

ANNIE is a Fortran program designed for mini- and microcomputers to help users interactively create, check, and update inputs to water-related models. ANNIE can be used to reformat, store, list, update, and plot data for models that require time-series information. ANNIE can be used to submit prepared model inputs to their respective models for processing. After model processing, ANNIE can also be used in the plotting and analysis of model results. At present, ANNIE is designed to work with the Hydrologic Simulation Program - Fortran (HSPF) and for the Precipitation/Runoff Model System. Limno-Tech has now adapted it to include interaction with DYNTOX. DYNTOX is contained wholly in the ANNIE package; it can only be accessed by running ANNIE.

The first step in accessing DYNTOX is to install ANNIE on the computer system to be used. If ANNIE has not yet been installed, this must be done before DYNTOX can be accessed. Installation of ANNIE and DYNTOX is described in the Appendix to this report.

Once the ANNIE program is installed and running, accessing DYNTOX is quite easy. ANNIE is designed to give the model user as much help as desired in choosing selections, and screens user responses for each question against acceptable values. For any section, the user need only enter "?" to find the acceptable range of responses. Figure 1 shows the initial portion of an example session with ANNIE for inexperienced users and Figure 2 for experienced users. User responses are denoted by arrows. Note that all user responses must be in capital letters. The first question determines how much help information is given to the user. The responses "NO", "LOTS", or "SOME" are acceptable for using DYNTOX. If the user specifies NO experience, he will be given the opportunity to view several paragraphs describing ANNIE. To stop this documentation, type NO when the prompt MORE? appears. The third question requires the response DYNTOX. (Only enough letters to distinguish your response from other acceptable responses is required). Users with experience using ANNIE will be prompted for information pertaining to User Control Input (UCI) files. This question is not relevant to the use of DYNTOX and the answer to this question should always be NO.

At this point in the session the DYNTOX programs are activated, and the user may choose from the three possible techriques: Continuous Simulation, Monte Carlo and Log Normal. A Complete description of program operations for the three techniques will be given in the subsequent sections, following a description of data required by all three techniques.

The user exits the DYNTOX session by selecting option 4, End Dynamic Toxics Analysis. There will again be a prompt concerning UCI files. The correct response to this question is DELETE (Figure 2).

```
#Execution begins
************************************************************
******            WELCOME TO "ANNIE"                  ******
******       VERSION DATED DECEMBER 5, 1984           ******
************************************************************
DO YOU HAVE NO, SOME, OR LOTS OF EXPERIENCE USING ANNIE?
NO
ANNIE helps prepare or update input to models.

Also, ANNIE helps create and fix the data for the time-series
     file (TSS file) that is used by some of the models.

Don't be concerned about bad entries,
     ANNIE guides you to acceptable responses.

When a question isn't clear, enter a question mark (?).

Many of the options are part of loops.  When you have finished
     all activities within a set of options, enter done to
     exit from the loop.
MORE?

NO
WHAT MODEL OR PROCESS DO YOU WANT TO USE?
?
HSPF        Simulation of hydrology using HSPF.
TSSMGR      Interactively create/add/modify/list TSS file.
STAT        Statistical analysis of time-series data.
PRMS        Simulation with Precip./Runoff Model System.
DR3M        Distributed Routing Rainfall/Runoff program.  **
CREAMS      US ARS rainfall/runoff model.  **
REFORMAT    Reformats USGS, NOAA, HSPF sequential files
            and adds data to TSS file from sequential files.
PLOT        Plots data from various sources to plotters.
DYNTOX      Dynamic Toxics Analyses.
            ** Not yet available.

Valid responses are:
HSPF      , TSSMGR     , STAT      , PRMS      , DR3M      , CREAMS     ,
REFORMAT  , PLOT       , DYNTOX

WHAT MODEL OR PROCESS DO YOU WANT TO USE?
DYNTOX
DYNAMIC TOXICS ANALYSES

WHICH TECHNIQUE DO YOU WANT TO USE:

 (1) CONTINUOUS SIMULATION: DILUTION AND DECAY
 (2) MONTE CARLO: DILUTION AND DECAY
 (3) LOG-NORMAL: DILUTION ONLY
 (4) END DYNTOX, RETURN TO ANNIE MENU

ENTER SELECTION (1-4)
(Hit return for 4)
4
```

FIGURE 1

Example Session with ANNIE (Inexperienced User)

```
 #Execution begins
 ****************************************************************
 ******            WELCOME TO "ANNIE"                      ******
 ******       VERSION DATED DECEMBER 5, 1984               ******
 ****************************************************************
 DO YOU HAVE NO, SOME, OR LOTS OF EXPERIENCE USING ANNIE?
> SOME
 WHAT MODEL OR PROCESS DO YOU WANT TO USE?
> DY
 ARE YOU WORKING FROM AN OLD UCI FILE?
> NO
 DYNAMIC TOXICS ANALYSES

 WHICH TECHNIQUE DO YOU WANT TO USE:

  (1) CONTINUOUS SIMULATION: DILUTION AND DECAY
  (2) MONTE CARLO: DILUTION AND DECAY
  (3) LOG-NORMAL: DILUTION ONLY
  (4) END DYNTOX, RETURN TO ANNIE MENU

 ENTER SELECTION (1-4)
 (Hit return for 4)
> 4
 SAVE, LIST, OR DELETE TEMPORARY UCI FILE
> D
#Execution Terminated
```

FIGURE 2

Example Session with ANNIE (Experienced User)

Upstream Boundary Data

DYNTOX requires data describing the daily river flow upstream of the effluent discharges. Data describing these flows are maintained for most rivers by the United States Geological Survey (USGS) and are available through STORET. Users should contact USGS State or District Office if they have questions about whether the flow record needs to be adjusted for point source inputs or water withdrawals. The first step in obtaining boundary flow data for DYNTOX is selecting the USGS gaging station to be used. The recommended location for the USGS gage is the closest gage upstream of the first discharge. Care should be taken to ensure that no major tributaries enter the river between the USGS gage and the first outfall. If no stations are available that meet the above criterion, the nearest gage downstream should be used. In this case, the user must enter the average point source flow or water withdrawals above the gage to correct the daily record for these effects. If the river is ungaged, it may be possible to use the flow record of a nearby river with similar drainage characteristics and proportion the daily flows by drainage area.

When the appropriate gage station has been selected, flow values can be retrieved using the FLOSTR option of STORET. Details for this procedure are contained in the STORET User Handbook (USEPA, 1982). The user must determine if the streamflow has been regulated by dams at any time before retrieving flow data for toxics analysis. This information is available in the Water Resources Data book published for each state by the USGS. If stream flow has been regulated, use only the data for the period which represents existing conditions.

STORET data are also often available for describing upstream concentration data. Since concentration data are usually taken at USGS gaging stations, the same station used for flow data should be used for concentration data. Unlike upstream flow, there are cases when STORET data for upstream concentrations cannot and should not be used. The first such case is when the USGS gage is located downstream of one of the modeled discharges. "Upstream" concentration data in this case would be biased by the effluent concentration and therefore not representative of conditions upstream of the discharge.

STORET data are not stored in toxic units and cannot be used for wasteload allocation modeling conducted using toxic units. In these cases the user must enter the data manually during program operation. Fortunately, in these cases a constant value will typically be used for upstream concentration. This value should be set to zero unless available data indicate that a different value is in order.

Concentration data is retrieved from STORET using the RETRIEVE command. Further documentation on STORET retrieval is located in the STORET User Handbook. Users can retrieve multiple parameters at one session; DYNTOX will prompt the user for the desired parameter during program operation.

System Data

Several types of information describing the river system are required. These include drainage area ratios from each outfall to the USGS gage, time of travel (velocity), withdrawals, and instream decay. The system data requirements are very similar between techniques and are discussed in this section. Specific examples of input for system data specific to each technique will be given later in their respective sections.

The drainage area ratio from each outfall to the USGS gage is required to determine the river flow immediately above each outfall by correcting for other flow inputs. This ratio should be determined by dividing the total drainage area for the river at the location of the outfall by the drainage area for the river at the USGS gage. When possible, a planimeter should be used to determine drainage areas.

Information on time of travel is required by the Continuous Simulation and Monte Carlo techniques for calculating instream fate processes (instream decay is not considered in the log normal analysis). Time of travel information is necessary to describe passage from the upstream boundary station to the first outfall and for the stretch of river between each outfall (in multiple discharge situations). Time of travel information can be obtained in one of two ways. First, dye studies can be conducted to determine the time of travel for each required stretch of river. Second, current meters can be used to calculate the average velocity in a reach. Time of travel information is determined from velocity measurements by dividing the length of the reach by the average velocity.

The user has two options for specifying time of travel. Time of travel may be described as constant or varying as a function of flow. Flow-dependent time of travel is recommended and is calculated by the equation:

$$\text{Time of Travel} = aQ^b \qquad (1)$$

where Q is river flow and a and b are constants. The coefficients a and b can be determined by plotting observed time of travel (distance/velocity) values at different flows on a log-log scale (Figure 3). The coefficient a is the y-intercept of the best fit line through the data, while b is the slope of the line. Note that b should be negative, as time of travel will decrease with increasing flow. Typical values for b range from -0.34 to -0.70 (Thomann, 1972). Constant time of travel requires only one input value that will be used for all flow conditions, and should be used when insufficient data are available to calculate flow-dependent time of travel.

The Continuous Simulation and Monte Carlo techniques in DYNTOX treat the instream fate of a toxic as a first-order decay and therefore require a first-order decay rate. Calculating this decay rate requires several data

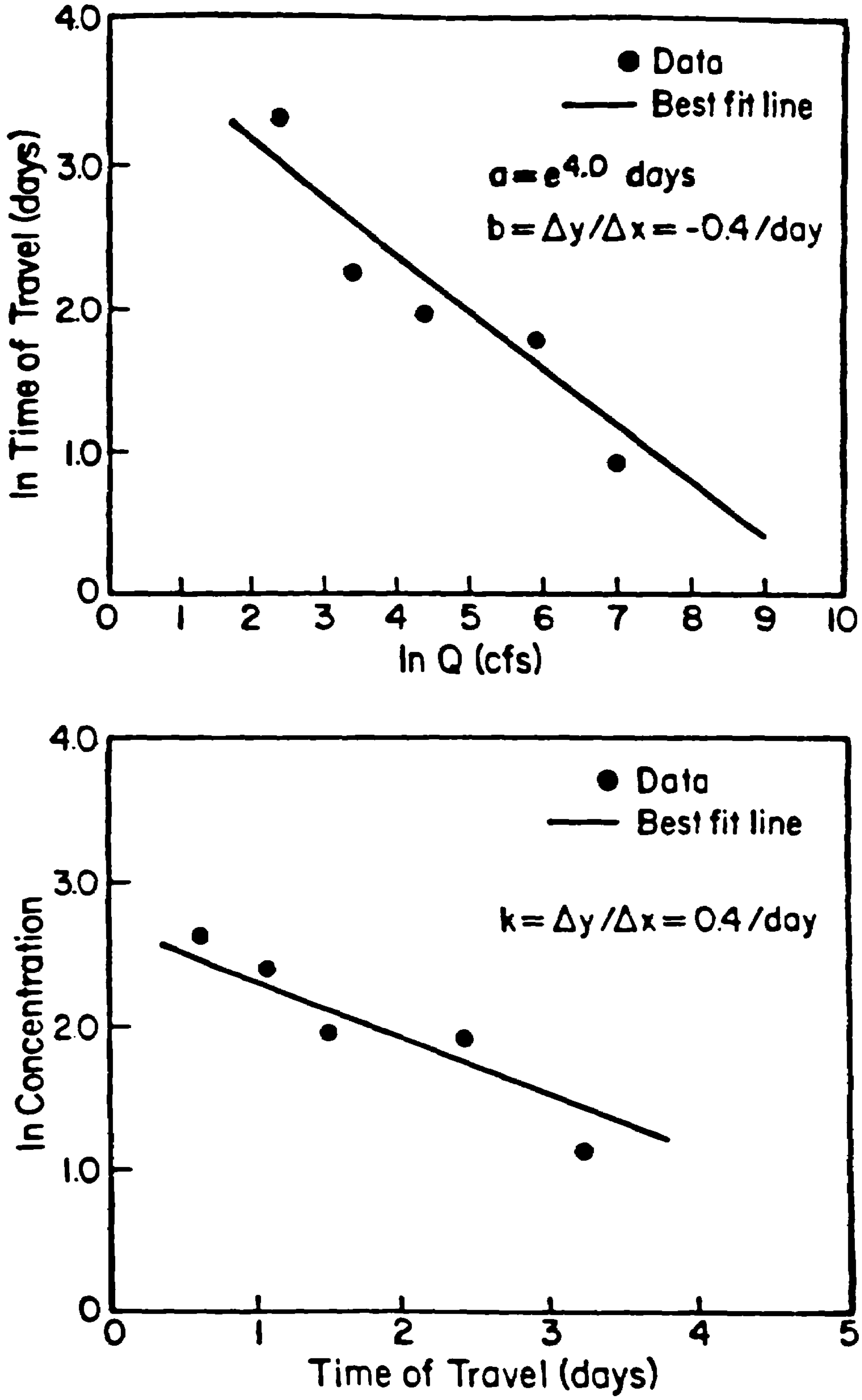

FIGURE 3

Determination of Input Constants

points taken from different stations on the river with a known time of travel and no pollutant sources between them. The natural logarithm of the concentration should be plotted versus time of travel (Figure 3) on semi-log paper and the decay rate calculated as the slope of the best fit line. This decay rate can change with changes in treatment for future scenarios. However, unless data are available to indicate otherwise, the same decay rate observed in-stream should be used for all wasteload allocation projections. When no in-stream data are available, the user should assume zero decay.

The user must also determine if there are significant water withdrawals (>1% of river flow) at any location over the stream section of interest. The average daily withdrawal rate will be prompted for in each river reach.

Effluent Data

Effluent data can be entered manually from the terminal during program operation or read from a previously created file. Required information consists of the total number of data points, and a date, flow, and concentration for each value. Care must be taken to use consistent units between river flow and concentration and effluent flow and concentration. That is, if river data have been entered using toxic units and cfs, effluent data must also be in toxic units and cfs.

III. CONTINUOUS SIMULATION

The most direct technique which can be used to simulate a probability distribution for instream toxics concentrations is Continuous Simulation. This technique directly predicts the concentration frequency distribution below an effluent discharge (or series of discharges) based on an observed history of upstream river flow and concentration. The Continuous Simulation technique has many advantages as it considers:

- frequency and duration of concentrations;
- instream fate and transport;
- single or multiple pollutant sources; and
- cross-correlation and serial correlation of parameters by using an actual historical sequence.

The primary disadvantage of the technique is that it requires a large and rostly complete set of data on historical conditions. Another disadvantage to Continuous Simulation is that computational requirements are significantly higher than for steady state modeling or for Log Normal analysis.

This chapter discusses the theory and application of the Cortinuous Simulation technique, and is divided into three sections. The first section discusses the theory upon which the model is based, and its advantages and disadvantages. The second section describes the data input requirements. The third and final section details how to use the computer model of the Continuous Simulation technique when performing waste load allocations.

Theory

As shown in Figure 4, a Continuous Simulation model uses model inputs for observed daily effluent flow (Q_e) and effluent concentration (C_e) and combines these with daily upstream receiving water flow (Q_u) and upstream concentration (C_u) to calculate downstream receiving water concentrations. The concentration directly below an effluent outfall (C_d) is determined from the equation:

$$C_d = \frac{Q_u C_u + Q_e C_e}{Q_u + Q_e} \qquad (2)$$

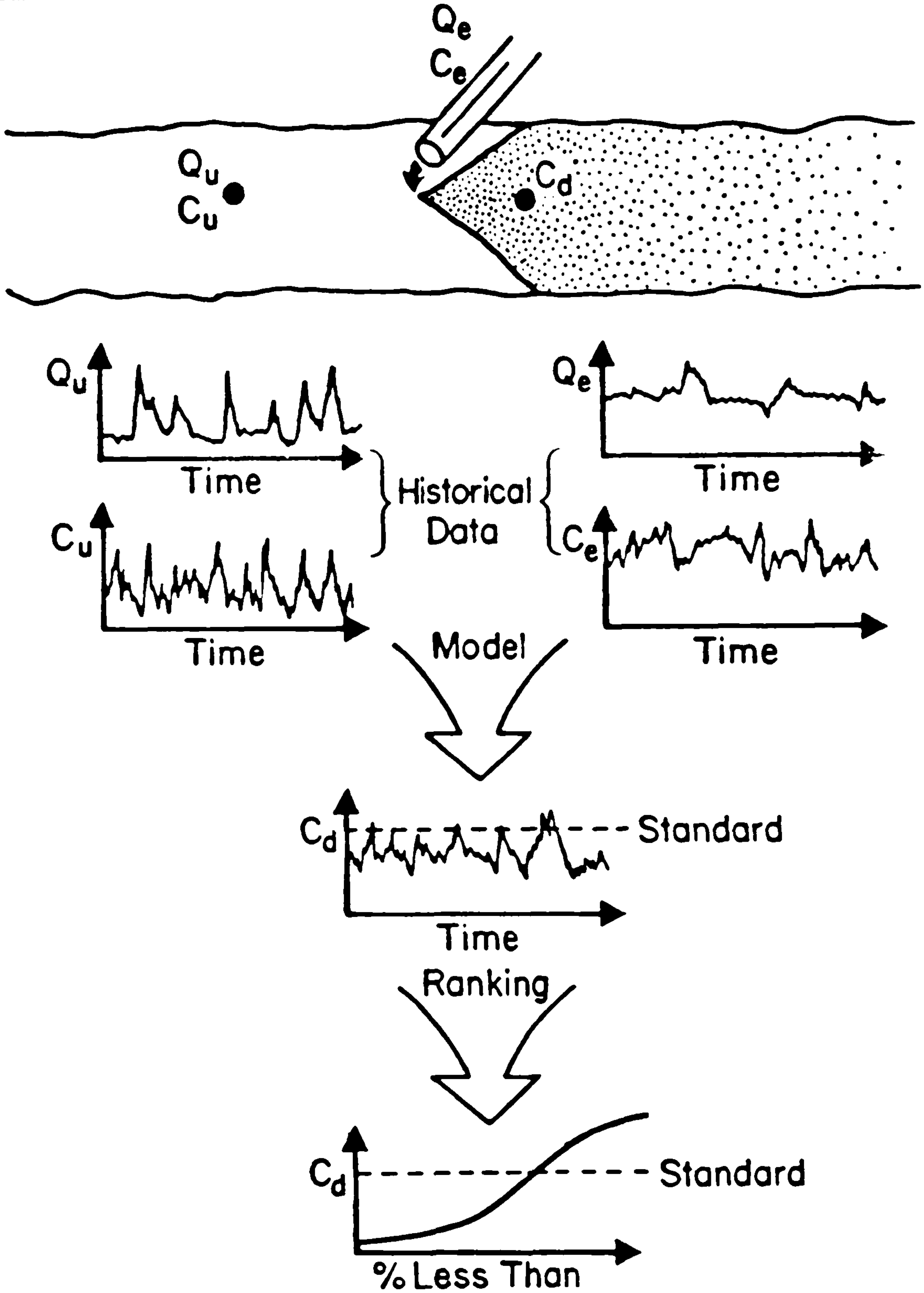

FIGURE 4

Continuous Simulation Modeling Schematic
(from USEPA 1984)

This technique assumes complete lateral mixing in the river. The model predicts a simulated history of instream concentrations in chronological order corresponding to the same time sequence of the model inputs.

The calculated daily downstream concentrations are ranked from the lowest to the highest without regard to time sequence. A probability distribution plot is constructed from these ranked values, and the recurrence frequency of any concentration of interest can be obtained (C_d vs. frequency). Running average concentrations for four days, or for any other averaging period, can also be computed from the simulated concentrations, ranked in order of magnitude, and also presented as a probability distribution (see Figure 5).

The Continuous Simulation model can predict the concentration below each of a series of discharges. Successive concentrations downstream are calculated progressively from the concentrations upstream on a day by day basis. Equation (2) is used to calculate the concentration downstream of the first discharge. The concentration further downstream but immediately upstream of the next discharge is calculated according to the following:

$$C_u = C_d * (e^{-kt}) \tag{3}$$

where: C_u = concentration above the second discharge
C_d = concentration below the first discharge
k = first-order decay rate
t = time of travel between discharges

The exponential term including the decay rate k represents any first order instream loss. Effects of subsequent discharges are calculated successively using equation (2) and (3). River flow above any particular discharge is the sum of the upstream boundary flow plus all additional flow inputs, including discharges.

The probability distribution plot generated by the Continuous Simulation technique will indicate the predicted frequency of criteria violations. These frequencies can be compared for different effluent alternatives. If evaluations of recurrence intervals of 10 or 20 years are desired, then at least 30 years of flow data should be available. This is needed to provide a sufficiently long record to estimate the probability of rare events. (The same data requirements are also true for the Log Normal and Monte Carlo methods).

The Continuous Simulation model has three primary advantages compared to steady state modeling, Monte Carlo and Log Normal analysis. First, the advantage over steady state modeling is that Continuous Simulation can predict the frequency and duration of toxicant concentrations in a receiving

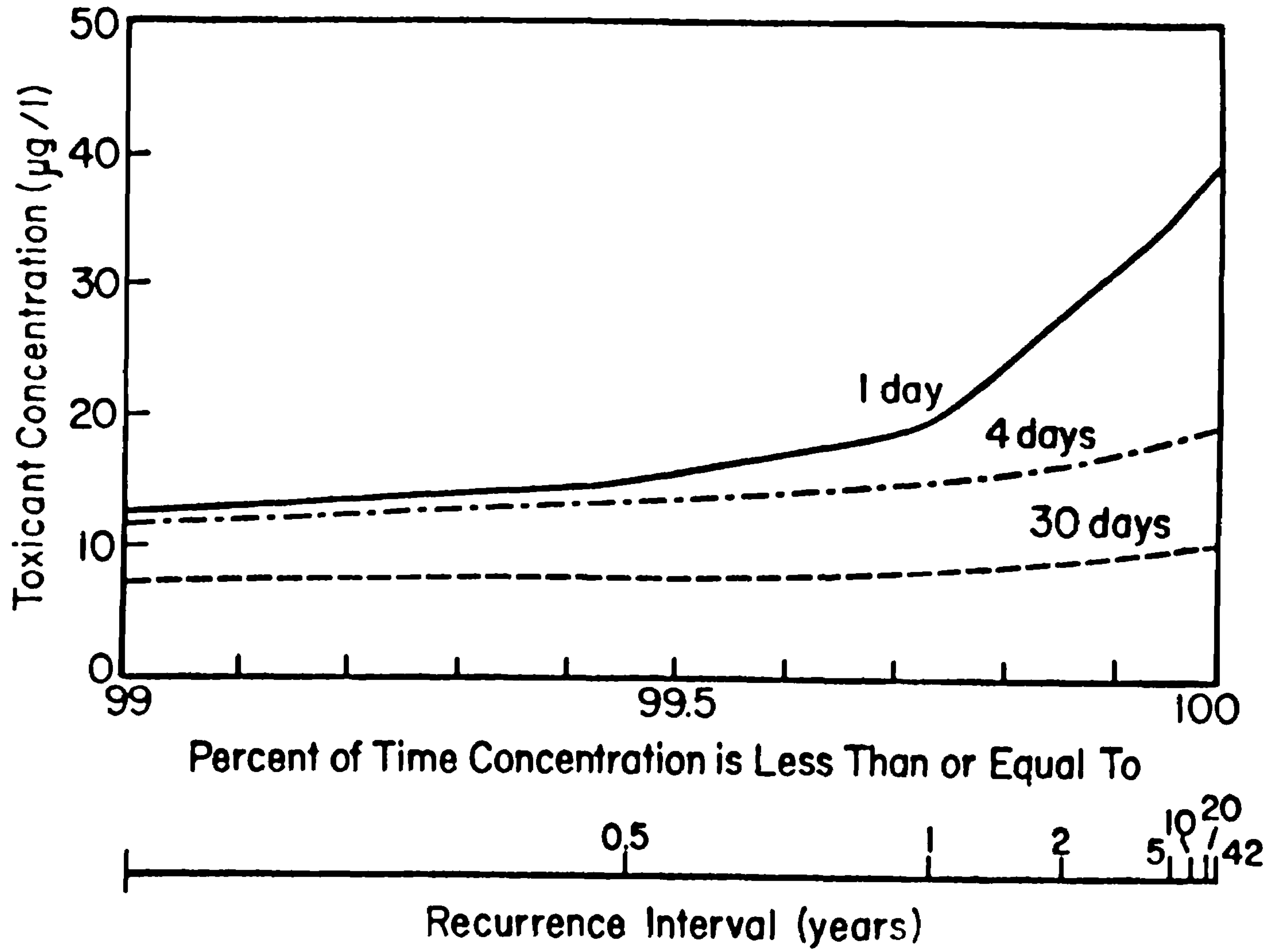

FIGURE 5

Concentration Frequency Curves
(from USEPA, 1984)

water; steady state analysis cannot. Second, the inclusion of instream fate processes is an advantage over Log Normal, which cannot simulate instream fate and is limited to simulations for one effluent discharge. Third, by using simultaneous observations for all input parameters, the Continuous Simulation model can directly incorporate the observed effects of serial and cross correlation of inputs. When calculating four day average instream concentrations, Continuous Simulation correctly does the averaging on the model results. Monte Carlo and Log Normal estimate four day average instream concentrations by averaging model inputs.

The primary disadvantage of Continuous Simulation is the large data requirement. A long period of historical data is required for all parameters. Although time series data can be synthesized for missing parameters, synthesis of time-series data for more than one parameter greatly reduces the reliability of this technique. Additional data are required for the calibration/verification of instream fate processes. A second disadvantage to Continuous Simulation is the large requirement of computer time and storage; however, recent advances in computer technology have minimized this problem.

Input Requirements

The model input requirements for all three techniques were discussed in Chapter 2. This section details the specific input requirements for the Continuous Simulation technique. The inputs can be generally categorized into four groups:

- o general simulation requirements,
- o upstream data,
- o effluent data, and
- o system physical and hydrologic constants.

All of these inputs are summarized in Table 1, and will be discussed individually in this section.

General Simulation Requirements: The Continuous Simulation method requires some general information on the system that will not change between simulations. The first basic input required for Continuous Simulation is to establish the period of the simulation. This consists of the beginning and the end date of the simulation, which must contain all or a portion of the streamflow record. This period should be as long as possible, since the power of the Continuous Simulation technique increases with the amount of observed data. The user should select a period for which a complete and consistent data set is available. Caution should also be directed against using old data which are no longer representative of current conditions.

	Data Source
o General Information:	
- Beginning and end date of simulation	USGS flow records
- Number of discharges above flow gage	User defined
- Average point source flow above gage	Treatment records
- TSS computer field name	User defined
o Upstream Data:	
- Time series flow data	STORET
- Data synthesis technique for flow	User defined
- Time series concentration data	STORET
- Data synthesis technique for concentration	User defined
o Effluent Data:	
- Time series flow data	Treatment records
- Data synthesis technique for flow	User defined
- Time series concentration data	Treatment records
- Data synthesis technique for concentration	User defined
o System Constants:	
- Time of travel information	Dye studies, current meters
- First order decay rate (s)	Instream data
- Drainage area ratio (s)	USGS topographic maps
- Water withdrawal rate (s)	Withdrawal records

Table 1. Input Requirements for the Continuous Simulation Technique

The second basic input required by Continuous Simulation is the number of discharges in the system. The user must also determine if any of these discharges are located upstream of the USGS gaging station; if so, the average point source flow above the gage must be determined in order to correct recorded streamflows for this input. The final general input required is a computer file name to store these inputs. Once these general inputs are specified, they will be stored in this computer file and need not be specified for later simulations.

Upstream Boundary Data: The Continuous Simulation technique requires time series information on upstream boundary flow and concentration, and effluent flow and concentration. The Continuous Simulation technique requires a data value for each individual day of the simulation. Typically many "holes" will exist in the data set, days which have no data for a given parameter. A method to synthesize or fill in data for missing days is required. Three methods are available for synthesizing missing data for the Continuous Simulation technique:

1. linear interpolation
2. simple Markov synthesis
3. multi-period Markov synthesis

Each is briefly described here as needed for use in this program. The reader is referred elsewhere for a more thorough theoretical discussion (Fiering and Jackson, 1971).

Linear interpolation is the simplest method. It synthesizes missing data by linearly interpolating between the available observed data values that bound the missing value. This method should be used in cases where data are available over the majority of the period of record and only minor "gaps" need to be filled in. When synthesizing missing upstream flow data, linear interpolation is the only method which should be used. Also, linear interpolation will produce a constant value repeated over the entire simulation when one observed data point exists.

The second method of data synthesis is a first-order, lag-one Markov process, referred to herein as simple Markov. With this technique, data for a given day are randomly determined from the overall data mean, overall data variance, the previous day's value, and an auto-correlation coefficient. The auto-correlation coefficient is a measure of how closely a given day's value is related to the previous day's value. The Markov process in DYNTOX assumes that daily fluctuations in model inputs are normally distributed. DYNTOX assumes an initial mean value and generates 50 data points in order to determine the first value used in the simulation. The only user input required by the simple Markov process is the auto-correlation coefficient. These coefficients can be determined using the SAS routine AUTOREG (SAS, 1982). A value for the auto-correlation coefficient of 0.7 is recommended if insufficient data are available for calculation from observed data. All other coefficients will be determined from the observed data by the program itself. The only exception is the case where less than three data values exist, in this situation the user must manually specify mean and variance or choose another method of data synthesis.

Multi-period Markov synthesis is the third technique and involves a third, more complex level of synthesis. The simple Markov process assumes that the process for which data is synthesized is "stationary" over the period of simulation; that is, the mean and variance remain relatively constant over the entire period of the simulation. The multi-period Markov process is designed to handle cases of non-stationary processes, where the mean and/or variance are known to change over time. The primary example of a non-stationary process is effluent flow from batch treatment. In this situation flow may be zero for several days during treatment, then non-zero for the next few days during discharge. The multi-period Markov process allows the user to divide a non-stationary process into as many repeating stationary periods as necessary. Each period requires data describing its mean value, standard deviation, and auto-correlation. These values must be calculated before performing a waste load allocation. Using the batch treatment flow as an example, the user would specify two periods to describe the process. The first period would have a mean and standard deviation of zero and a length equal to the duration of the treatment period. The second period would have an appropriate mean and standard deviation and a length equal the duration of the discharge. DYNTOX then uses a Markov process to repeat the two periods until a data value for each day is generated.

Effluent Data: Similar to upstream data, daily input values are needed in the model for effluent flow and concentration (or toxicity). The source of these data must be user specified. As for the upstream data, gaps are likely to exist in any data set. Here again, the user must use either linear interpolation, simple Markov, or multi-period Markov to synthesize data for missing days. Any downstream tributary inputs occurring between discharges should be considered as a separate effluent input.

System Constants: System constants need to be defined for hydrologic and physical characteristics of the system. Model inputs for physical data include time of passage between locations and instream loss rates. Time of passage must be defined for the stream segment between the upstream boundary station and the first discharge, as well as for the segments between each discharge. The coefficients used to define the time of passage were discussed previously in the Common Requirements chapter. Instream losses are defined by a first-order decay rate, and are held constant in each reach throughout the simulation period. The method for determining the first-order decay rate was also discussed in the Data Requirements chapter.

Program inputs for hydrologic data are needed to properly adjust gauged flow data to determine instream flow at different locations. Ratios are needed to define the comparison between the gauged drainage basin area and the drainage basin area at the point of discharge. These ratios adjust the USGS measured flows for non-point sources, and must be specified regardless of the location of the gaging station. For discharges located downstream of the USGS gage the ratio (and adjustment) will be greater than 1.0. For discharges located upstream of the gage, the ratio will be less than 1.0. The method to be used for specifying drainage area ratios is described in the Common Requirements chapter. A second hydrologic adjustment is required for water withdrawals. If a significant amount of water (>1% of river flow) is withdrawn from the river at any location, this withdrawal rate must be specified before performing a Continuous Simulation waste load allocation.

Program Use

The Continuous Simulation program, like the programs for the other techniques, is divided into menu driven sub-programs (entitled activities) to allow the user as much flexibility as possible in performing simulations. The hierarchy of activities for Continuous Simulation is shown in Figure 6. This section will describe how to use the Continuous Simulation program and will discuss the options available. It is divided into sections describing each of the primary activities of Continuous Simulation:

- o Program Entry,
- o Input Specification,
- o Model Simulation,
- o Viewing/Analysis of Input Data,
- o Viewing/Analysis of Simulation Results, and
- o Ending Continuous Simulation

Program Entry: The first activity of the Continuous Simulation technique is termed Program Entry. This section involves either the initialization and development of the basic input file or the specification of an existing file. Initial data include those data and information which typically would not be changed in alternative simulations. They include the period of data record (duration of simulation), the number of discharges, and the data base used to define upstream flows and concentration. Modifications to the data including data interpolation, loss rates, and effluent inputs are handled in another activity (entitled Input Specification) because these factors may be changed in alternative simulations.

Figure 7 shows example sessions with the Program Entry activity. The first questions in Program Entry concerns the existence and location of the TSS files used for the simulation. Time Series Store (TSS) files are created by ANNIE to hold all time series information for a system, such as the period of simulation and observed flow and concentration data for upstream

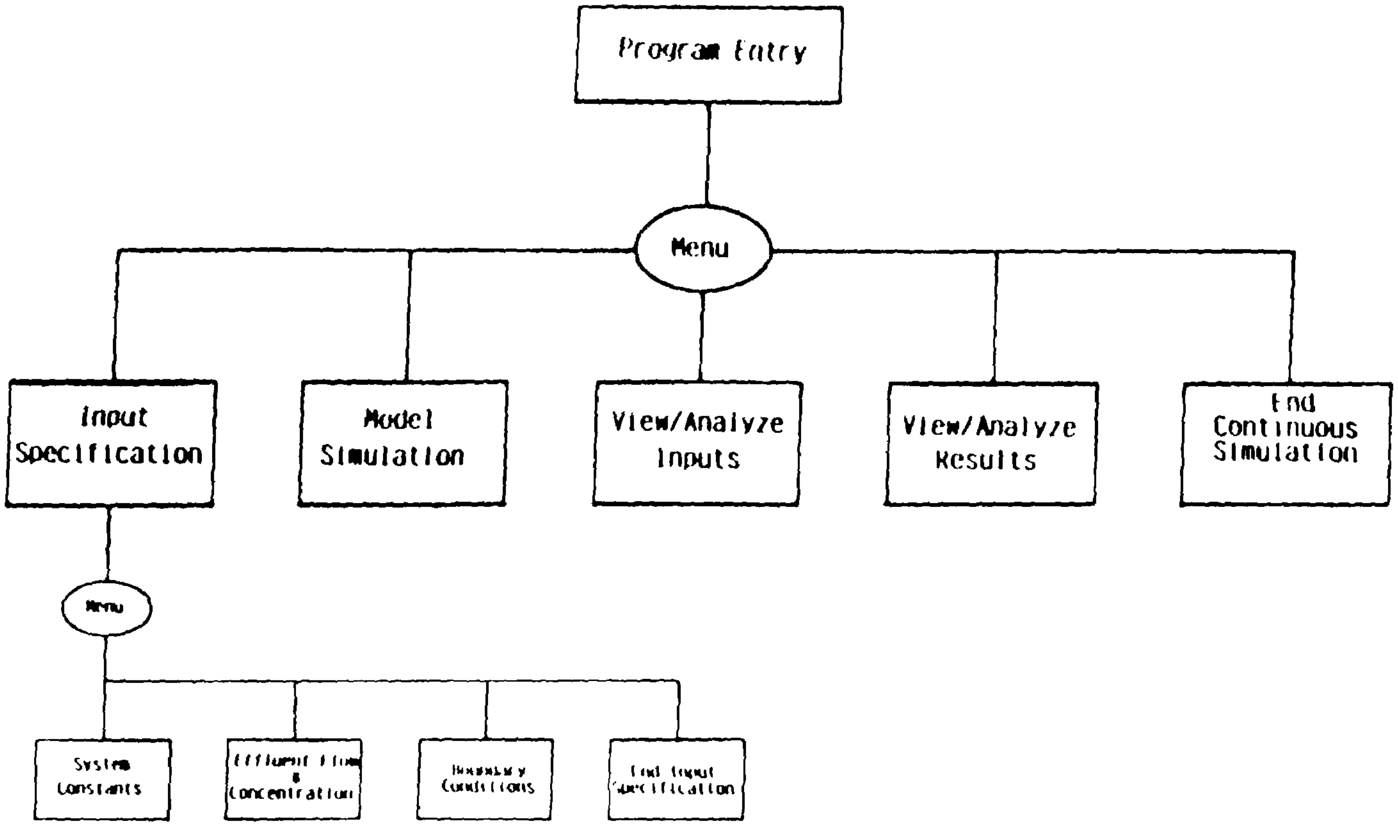

FIGURE 6

Hierarchy of Continuous Simulation Subprograms

7a. New TSS File

```
      DYNAMIC TOXICS ANALYSES

      WHICH TECHNIQUE DO YOU WANT TO USE:

       (1) CONTINUOUS SIMULATION: DILUTION AND DECAY
       (2) MONTE CARLO: DILUTION AND DECAY
       (3) LOG-NORMAL: DILUTION ONLY
       (4) END DYNTOX, RETURN TO ANNIE MENU
      ENTER SELECTION (1-4)
      (Hit return for 4)
  ➤   1
      HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
  ➤   NO
      WHAT IS THE NAME OF YOUR NEW TSS FILE?
  ➤   EXAMPLE
      ENTER BEGINNING AND ENDING DATES FOR SIMULATION:
      ENTER STARTING DATE.
  ➤   1980/1/1
      ENTER ENDING DATE.
  ➤   1980/12/31
      HOW MANY OUTFALLS ARE THERE IN THE SYSTEM?
      (Hit return for 1)
  ➤   1
      HOW MANY OUTFALLS LIE ABOVE THE FLOW GAGE?
      (Hit return for 0)
  ➤   0
      PLEASE WAIT WHILE YOUR TSS FILE IS INITIALIZED ...

      INITIALIZATION OF YOUR TSS FILE IS NOW COMPLETE.

      DO YOU HAVE A STORET FLOW DATA FILE?
  ➤   Y
  ➤   WHAT IS THE NAME OF THE STORET FILE?
      STORET.FLO
      USE WHICH DATA SET?
      (Hit return for 1)
  ➤   1
      WHAT IS THE MAXIMUM ACCEPTABLE FLOW VALUE?
      (Hit return for 0.)
  ➤   4999.
       6265 POINTS READ

      DO YOU HAVE A STORET DATA FILE FOR UPSTREAM CONCENTRATION?
  ➤   YES
      WHAT IS THE NAME OF THE STORET FILE?
  ➤   STORET.CON
      USE WHICH DATA SET?
      (Hit return for 1)
  ➤   1
      WHAT IS THE MAXIMUM CONCENTRATION VALUE?
      (Hit return for 0.)
  ➤   1.0
       1156 POINTS READ
```

FIGURE 7

Example Session with Continuous Simulation Program Entry

7b. Existing TSS File

```
      ENTER SELECTION (1-4)
      (Hit return for 4)
   ➤  1
      HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
   ➤  YES
      WHAT IS THE NAME OF YOUR TSS FILE?
   ➤  EXAMPLE
```

7c. Terminal Entry of Data

```
      HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
   ➤  NO
      WHAT IS THE NAME OF YOUR NEW TSS FILE?
   ➤  EXAMPLE
      ENTER BEGINNING AND ENDING DATES FOR SIMULATION:
      ENTER STARTING DATE.
   ➤  196[illegible]
      ENTER ENDING DATE.
   ➤  198[illegible]/12/31
      HOW MANY OUTFALLS ARE THERE IN THE SYSTEM?
      (Hit return for 1)
   ➤  1
      HOW MANY OUTFALLS LIE ABOVE THE FLOW GAGE?
      (Hit return for 0)
   ➤  0

      PLEASE WAIT WHILE YOUR TSS FILE IS INITIALIZED ...

      INITIALIZATION OF YOUR TSS FILE IS NOW COMPLETE.

      DO YOU HAVE A STORET FLOW DATA FILE?
   ➤  Y
      WHAT IS THE NAME OF THE STORET FILE?
      STORET.FLO
      USE WHICH DATA SET?
      (Hit return for 1)
   ➤  1
      WHAT IS THE MAXIMUM ACCEPTABLE FLOW VALUE?
      (Hit return for 0.)
   ➤  4999.
       6245 POINTS READ

      DO YOU HAVE A STORET DATA FILE FOR UPSTREAM CONCENTRATION?
   ➤  NO
      DO YOU WANT TO ENTER CONCENTRATION DATA FROM THE TERMINAL?
   ➤  YES
      HOW MANY SAMPLES DO YOU HAVE?
      (Hit return for 4)
   ➤  3

      ENTER DATE AND UPSTREAM CONCENTRATION FOR EACH SAMPLE:
   ➤  600101, .5
   ➤  601231, .4
   ➤  650615, .23
           3 POINTS READ
```

FIGURE 7 Cont'd.

Example Session with Continuous Simulation Program Entry

```
CONTINUOUS SIMULATION TECHNIQUE

   PLEASE CHOOSE FROM THE FOLLOWING:

   (1) SPECIFY MODEL INPUTS
   (2) RUN THE SIMULATION
   (3) VIEW/ANALYZE THE INPUT DATA
   (4) VIEW/ANALYZE THE SIMULATION RESULTS
   (5) END CONTINUOUS SIMULATION

   ENTER YOUR CHOICE (1 - 5):
(Hit return for 1)
➤ 1


PREPARE MODEL INPUT TIMESERIES

   (1) SPECIFY SYSTEM CONSTANTS
   (2) SPECIFY OUTFALL FLOWS AND CONCENTRATIONS
   (3) READ UPSTREAM BOUNDARY FLOWS AND CONCENTRATIONS
   (4) END TIMESERIES DEFINITION AND RETURN TO CONTINUOUS
       SIMULATION MENU

   ENTER YOUR CHOICE (1 - 4):
(Hit return for 1)
➤ 1
   ----- SYSTEM CONSTANTS -----

   INPUT DATA FOR EACH REACH


SYSTEM CONSTANTS FOR REACH 1, BETWEEN UPSTREAM BOUNDARY AND FIRST OUTFALL
   HOW DO YOU WANT TO SPECIFY THE TIME OF TRAVEL?

   (1) CONSTANT
   (2) AS A FUNCTION OF FLOW

   ENTER YOUR CHOICE (1 OR 2):
(Hit return for 1)
➤ 1
WHAT IS THE TIME OF TRAVEL IN DAYS
(Hit return for 0.1)
➤ .1
   WHAT IS THE FIRST ORDER DECAY RATE?
(Hit return for 0.1)
➤ .1
   WHAT IS THE AVERAGE WITHDRAWAL?
➤ 0.
   WHAT IS THE DRAINAGE AREA RATIO FROM THE USGS GAGE?
(Hit return for 1.)
➤ 1.
```

FIGURE 8

Example Session with Continuous Simulation System Constants conditions. The first time a simulation is performed the user should answer NO to the question asking if a TSS file was previously created (Figure 7a). This will initiate the process to create a file. The user should answer YES to this question in subsequent simulations, and no other information will be required in the Program Entry section (Figure 7b).

For first time entries, the TSS file name must be supplied. Any file name can be used that is compatible with the computer system. The next inputs required are the beginning and end dates of the simulation which define the extent of the input data base. The required format for these dates are Year/Month/Day. Months and days with only one significant figure of information may be entered using one digit. Four digits are needed to define the year. The last question before creation of the TSS file concerns the number of discharges in the system.

At this point in Program Entry, the TSS file for the system is being created and initialized. This may take some time, depending on the computer system used, but the user will be informed when the file initialization is complete. TSS files created during Continuous Simulation can be used for either of the three interactive programs contained in DYNTOX.

The final portion of Program Entry concerns defining the upstream boundary data files. Figure 7a shows an example session where both the boundary flow and boundary concentration data are located in STORET files. The user need only specify the location of the STORET data file and which data set of the STORET retrieval is desired. The data set number selected by the user should be one, unless multiple data sets were stored in the same file during the STORET retrieval. This section also provides the ability to correct the STORET data and screen out flow and concentration values above acceptable values. Observed data above the maximum acceptable value are set to this cut-off value.

The final possibility for Program Entry is when the user has no STORET data and wishes to enter observed flow and concentration data manually from the terminal. Figure 7c shows an example of this situation. The user is required to input the number of data values and then the date and concentration for each value. The proper format is date and value with the date being in the YYMMDD (two digits for year, two digits for month, two digits for day) format.

After completing Program Entry, the program enters the main portion of the Continuous Simulation program. The user will be given the menu shown in Figure 9 and must select one of the five activities:

1. Input Specification
2. Model Simulation
3. View/Analyze Inputs
4. View/Analyze Results
5. End Simulation

Although there is some flexibility in the order in which activites are selected, inputs must be specified before choosing any other option (except ending).

Input Specification: Selecting Input Specification provides a new menu involving four subtasks: 1) System constants, 2) Effluent flow and concentrations, 3) Boundary condition data, and 4) Ending input specifications. These four tasks can be selected in any order desired.

The first task of input specification pertains to the system constants: time of travel, first-order loss rate, drainage area ratio, and water withdrawal rate. Program operation for this task is very straightforward, requiring only the inputs discussed in the data requirement section. An example session specifying system constants is shown in Figure 8.

The second subtask of input specification covers effluent flows and concentrations (Figure 9). The user has the option of entering data directly from the terminal or having the data read from a file. The required format in both cases is the number of data points followed by the date, flow, and concentration for each observation on a line separated by commas. The proper format for the date is YYMMDD.

Next, the user must specify the desired data synthesis technique used to define data values missing in the input data file. This method is selected first for effluent flow and then for effluent concentration. The specifics of the data synthesis techniques were described in the Upstream Boundary Data section of this chapter. The implementation of these three techniques is quite simple. For linear interpolation (see Figure 9a), no additional user inputs are required. The first-order Markov process requires user specification only of the auto correlation coefficient (Figure 9a) since the program internally computes the mean and standard deviation of the data. The user has the ability to calculate coefficients from the data or to override the statistics and input any selected values. Where sufficient data are not available for the program to calculate statistics, the user must manually specify statistics or choose a new technique. The multiple-period Markov process requires somewhat more user input than the other data synthesis techniques (see Figure 9b). The first input is the number of repeating periods to be used. For each repeating period, the user must manually specify the mean value, standard deviation, and auto-correlation coefficient.

The boundary data task involves completing the input data file for upstream flow and concentration. This also requires the selection of a technique to fill in missing data. The program requires specification of a data synthesis technique both for boundary concentration and flow. The same procedure used for synthesis of effluent data applies for synthesis of boundary data. Linear interpolation should always be selected as the data synthesis technique for boundary flow, since a thorough boundary flow data set is essential to the proper function of Continuous Simulation.

9a. Linear Interpolation and Simple Markov

```
        PREPARE MODEL INPUT TIMESERIES

           (1) SPECIFY SYSTEM CONSTANTS
           (2) SPECIFY OUTFALL FLOWS AND CONCENTRATIONS
           (3) READ UPSTREAM BOUNDARY FLOWS AND CONCENTRATIONS
           (4) END TIMESERIES DEFINITION AND RETURN TO CONTINUOUS
               SIMULATION MENU

           ENTER YOUR CHOICE (1 - 4):
        (Hit return for 1)
    ➤  2
        IS YOUR EFFLUENT DATA IN A FILE?
    ➤  NO

        DISCHARGE #   1
        HOW MANY POINTS DO YOU HAVE FOR THIS DISCHARGE?
        (Hit return for 4)
    ➤  3
        ENTER DATE, FLOW, AND CONCENTRATION FOR EACH SAMPLE:
    ➤  600202, 25., 1.
    ➤  600404, 23., .8
    ➤  600503, 26., .7
             3 POINTS READ

        DATA SYNTHESIS FOR EFFLUENT FLOW

        WHAT TECHNIQUE DO YOU WANT TO USE TO SYNTHESIZE MISSING DATA
        (1) LINEAR INTERPOLATION (OR CONSTANT VALUE)
        (2) FIRST ORDER MARKOV
        (3) MULTIPLE PERIOD MARKOV
        ENTER 1-3
        (Hit return for 1)
    ➤  1

        DATA SYNTHESIS FOR EFFLUENT CONCENTRATION

        WHAT TECHNIQUE DO YOU WANT TO USE TO SYNTHESIZE MISSING DATA
        (1) LINEAR INTERPOLATION (OR CONSTANT VALUE)
        (2) FIRST ORDER MARKOV
        (3  MULTIPLE PERIOD MARKOV
        ENTER 1-3
        (Hit return for 1)
    ➤  2
        MEAN VALUE IS  0.83333
        STANDARD DEVIATION IS  0.15275
        IS THIS ACCEPTABLE?
    ➤  Y
        WHAT IS THE AUTO-CORRELATION COEFFICIENT FOR THIS PARAMETER
        (Hit return for 0.)
    ➤  .7
```

FIGURE 9

Example Session with Continuous Simulation Effluent Specification

9b. Multiple Period Markov

```
      DATA SYNTHESIS FOR EFFLUENT FLOW

      WHAT TECHNIQUE DO YOU WANT TO USE TO SYNTHESIZE MISSING DATA
      (1) LINEAR INTERPOLATION (OR CONSTANT VALUE)
      (2) FIRST ORDER MARKOV
      (3) MULTIPLE PERIOD MARKOV
      ENTER 1-3
      (Hit return for 1)
  ➤
      PARAMETER SPECIFICATION FOR MULTIPLE PERIOD MARKOV PROCESS

      HOW MANY REPEATING PERIODS DO YOU WANT TO USE
      (Hit return for 2)
  ➤   2
      DESCRIBE PERIOD   1
      HOW MANY DAYS IN THIS PERIOD
      (Hit return for 10)
  ➤   10
      WHAT IS THE MEAN VALUE FOR THIS PERIOD
      (Hit return for 1.)
  ➤   25.
      WHAT IS THE STANDARD DEVIATION FOR THIS PERIOD
      (Hit return for 0.)
  ➤   3.
      WHAT IS THE AUTO-CORRELATION COEFFICIENT DURING THIS PERIOD
      (Hit return for 0.)
  ➤   .7
      DESCRIBE PERIOD   2
      HOW MANY DAYS IN THIS PERIOD
      (Hit return for 10)
  ➤   3
      WHAT IS THE MEAN VALUE FOR THIS PERIOD
      (Hit return for 1.)
  ➤   .01
      WHAT IS THE STANDARD DEVIATION FOR THIS PERIOD
      (Hit return for 0.)
  ➤   .001
      WHAT IS THE AUTO-CORRELATION COEFFICIENT DURING THIS PERIOD
      (Hit return for 0.)
  ➤   .7
```

FIGURE 9 Cont'd.

Example Session with Continuous Simulation
Effluent Specification

The final task of input specification is to end and return to the main Continuous Simulation menu. This option may be selected at any time; however, to run a simulation the previous three options must all be successfully executed.

Model Simulation: The model simulation can be conducted any time after the inputs have been fully specified. No additional inputs are required to run the simulation. The program will print out each 500 days of program execution as they are completed so the user can monitor program progress.

View/Analyze Inputs: The user has the ability to view any of the model input parameters in either tabular or graphic format using any averaging period (1-day, 4-day, etc.). This activity can be accessed any time after the inputs have been specified, but need not be conducted. After specifying the parameter to be viewed, an averaging period must be supplied. The user then has the option of selecting a table (Figure 10) and/or a plot (Figure 11) of inputs.

Graphical plots of model inputs show the percentage of the input values for a particular parameter that occurs in each of ten value ranges. Tabular results give a statistical evaluation of the parameter of interest in terms of mean value, standard deviation and coefficient of variation. The tabular presentation also shows the percentage of the data that exceeds various values, the return period (recurrence interval) for exceeding these limits, and the percentage of the data occurring between various limits. Additional features of tabular results are the ability to determine the return period for any value of interest and the ability to view the value that has exactly a three year return period.

View/Analyze Results: This activity of the program can be accessed any time after a simulation has been run. The format for the activity is identical to that for the viewing/analysis of inputs. The results shown indicate the frequency distribution for the in-stream concentration directly at the point of mix with the specified discharge (Figure 12). Tabular results are identical to the view/analyze inputs activity section.

End Continuous Simulation: The final option of the Continous Simulation program is to end and return to the main DYNTOX menu. This option may be selected at any time during the session.

```
CONTINUOUS SIMULATION TECHNIQUE

   PLEASE CHOOSE FROM THE FOLLOWING:

   (1) SPECIFY MODEL INPUTS
   (2) RUN THE SIMULATION
   (3) VIEW/ANALYZE THE INPUT DATA
   (4) VIEW/ANALYZE THE SIMULATION RESULTS
   (5) END CONTINUOUS SIMULATION

   ENTER YOUR CHOICE (1 - 5):
(Hit return for 1)
3


VIEWING ANALYSIS OF INPUTS

   WHICH PARAMETER DO YOU WANT TO VIEW?

   (1) OUTFALL DISCHARGE
   (2) OUTFALL CONCENTRATION
   (3) UPSTREAM BOUNDARY DISCHARGE
   (4) UPSTREAM BOUNDARY CONCENTRATION

   ENTER YOUR CHOICE (1 - 4):
(Hit return for 1)
2
   WHICH OUTFALL IS OF INTEREST (ENTER OUTFALL NUMBER)?
(Hit return for 1)
2
        ENTER AVERAGING PERIOD (IN DAYS):
(Hit return for 1)
3
DO YOU WANT TO SEE A PLOT?
N
DO YOU WANT TO SEE A STATISTICS TABLE?
Y

WHAT TITLE DO YOU WANT FOR YOUR TABLE (80 CHARACTER MAXIMUM)
STATISTICS TABLE
```

FIGURE 10

Example Tabular Display of Continuous Simulation Inputs

STATISTICS TABLE

MEAN = 6.530 STANDARD DEVIATION = 2.400
COEFFICIENT OF VARIATION = 0.264

VALUE	% OF TIME EXCEEDED	% OF TIME IN INTERVAL	RETURN PERIOD (YEARS
0.0	100.000		0.003
		0.0	
2.50	100.000		0.003
		10.929	
5.00	89.071		0.003
		23.497	
7.50	65.574		0.004
		43.169	
10.0	22.404		0.012
		19.126	
12.5	3.279		0.084
		3.279	
15.0	0.0		-999.000
		0.0	
17.5	0.0		-999.000
		0.0	
20.0	0.0		-999.000
		0.0	
22.5	0.0		-999.000
		0.0	
25.0	0.0		-999.000

DO YOU WANT TO: (1) SEE A RETURN PERIOD FOR A DIFFERENT VALUE
(2) CALCULATE THE VALUE WITH A THREE YEAR RETURN PERIOD
OR (3) END TABULAR ANALYSIS
3
ENTER VALUE
(Hit return for 1.)
11.
THE RETURN PERIOD FOR 11.00 IS 0.02 YEARS

FIGURE 10 Cont'd.

Example Tabular Display of Continuous Simulation Inputs

```
   VIEWING ANALYSIS OF INPUTS

      WHICH PARAMETER DO YOU WANT TO VIEW?

      (1) OUTFALL DISCHARGE
      (2) OUTFALL CONCENTRATION
      (3) UPSTREAM BOUNDARY DISCHARGE
      (4) UPSTREAM BOUNDARY CONCENTRATION

      ENTER YOUR CHOICE (1 - 4):
   (Hit return for 1)
➤  2
      WHICH OUTFALL IS OF INTEREST (ENTER OUTFALL NUMBER)?
   (Hit return for 1)
➤  2
           ENTER AVERAGING PERIOD (IN DAYS):
   (Hit return for 1)
➤  3
   DO YOU WANT TO SEE A PLOT?
➤  Y
   INTERVAL OF CUMULATIVE FORMAT
➤  I
   WHAT TITLE DO YOU WANT FOR YOUR PLOT (80 CHARACTER MAXIMUM)
   EFFLUENT CONCENTRATION
```

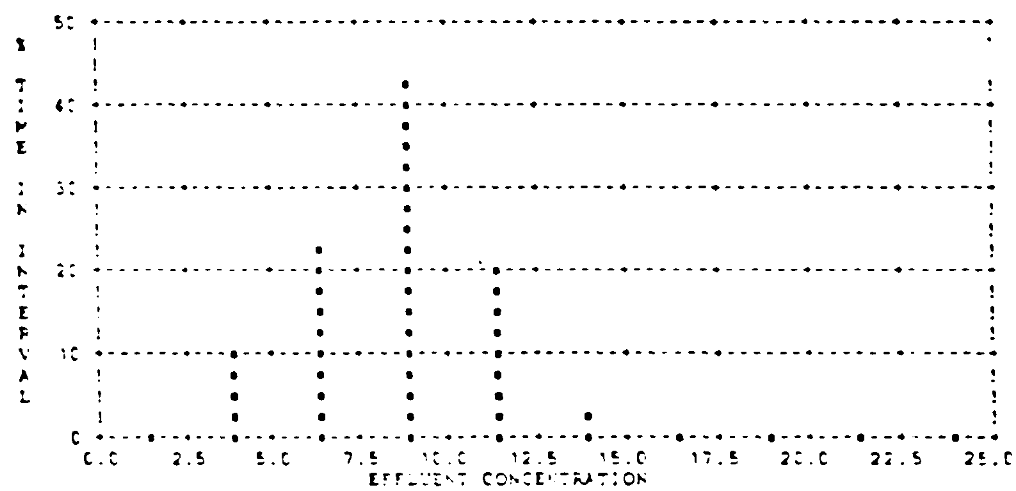

FIGURE 11

Example Plot Display of Continuous Simulation Inputs

```
CONTINUOUS SIMULATION TECHNIQUE

   PLEASE CHOOSE FROM THE FOLLOWING:

   (1) SPECIFY MODEL INPUTS
   (2) RUN THE SIMULATION
   (3) VIEW/ANALYZE THE INPUT DATA
   (4) VIEW/ANALYZE THE SIMULATION RESULTS
   (5) END CONTINUOUS SIMULATION

   ENTER YOUR CHOICE (1 - 5):
(Hit return for 1)
4

VIEWING/ANALYSIS OF RESULTS

        ENTER AVERAGING PERIOD (IN DAYS):
(Hit return for 1)
1
DO YOU WANT TO SEE A PLOT?
Y
WHAT TITLE DO YOU WANT (80 CHARACTER MAXIMUM)
CONTINUOUS SIMULATION CONCENTRATION
```

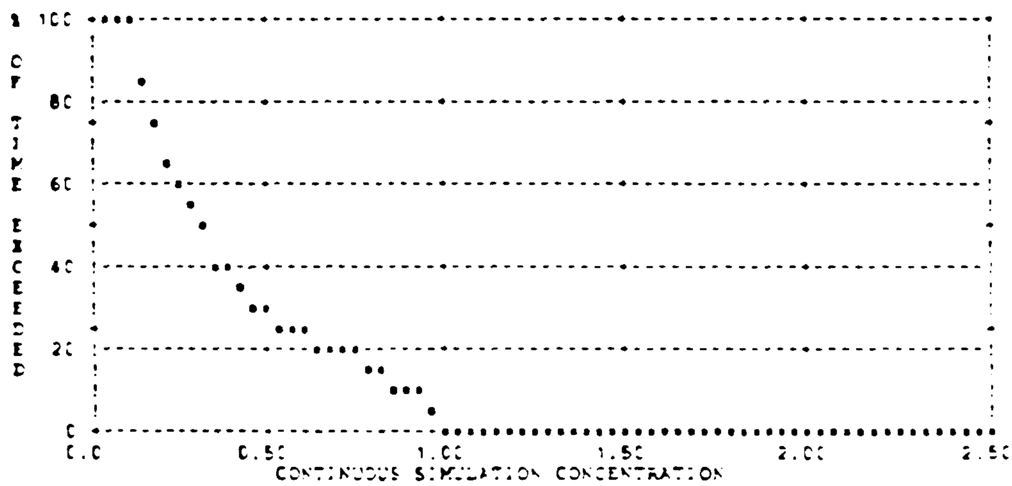

FIGURE 12

Example Plot Display of Continuous Simulation Results

IV. MONTE CARLO

The second technique which can be used to simulate a probability distribution for instream toxics concentrations is Monte Carlo simulation. This technique combines probabilistic and deterministic analyses, by using a fate and transport mathematical model with statistically described model inputs. The Monte Carlo simulation technique has many advantages as it:

- o calculates frequency and duration of toxicant concentrations;
- o includes instream fate and transport processes;
- o simulates single or multiple pollutant sources;
- o requires less extensive data than Continuous Simulation;
- o model inputs need not follow a specific statistical function;
- o incorporates cross and serial correlation.

The primary disadvantage to Monte Carlo is that it still requires extensive input data to define probability distributions for inputs. If extensive data are not available, the user must have enough information to assume distributions for the input parameters.

This chapter discusses the theory and application of the Monte Carlo technique, and is divided into three sections. The first section discusses the theory upon which the model is based, its advantages and disadvantages. The second section describes the data input requirements. The third and final section details how to use the computer model of the Monte Carlo simulation technique when performing waste load allocations.

Theory

Ordinarily, deterministic water quality simulations use single values for inputs to conduct a single steady state model simulation, providing a single water quality prediction. Single values are selected for upstream flow, upstream concentration, effluent flow, effluent concentration and decay rate. The model is then used to simulate a single water quality response profile. In multiple discharge cases, the concentration above each outfall is determined from the concentration below the previous outfall. Equations 2, 3 and 4 in Chapter 3 detail the mathematics involved. These equations are appropriate for all river modeling cases except mixing zone anaylsis.

The Monte Carlo technique is similar to the above, but repeats the simulation many times. It repetitively selects model inputs according to defined statistical distributions. The deterministic model is repetitively run for a large number of statistically selected sets of inputs. Results when summarized (see Figure 13) show a range of predicted concentrations at each stream location. This range reflects the range of possible input conditions and outcomes for the model. The range in predicted concentrations is characterized by a distribution. This distribution indicates the probabilities of concentrations over the entire range.

By combining statistical information on environmental conditions with deterministic model calculations, a statistically predicted forecast of water quality is obtained. The input distibutions statistically reflect our best understanding of model inputs. The predicted concentration distributions, therefore, reflect the best estimate of the range in predicted water quality conditions. Analysis of this distribution can provide information on the probability of water quality problems and their severity. For a more in-depth discussion of using Monte Carlo to perform waste load allocations, the user is referred to Freedman and Canale (1983).

The Monte Carlo technique has several advantages over steady state modeling and the non-steady state techniques Continuous Simulation and Log Normal Analysis. The main advantage over steady state modeling is that Monte Carlo can predict the frequency and duration of toxicant concentrations in a receiving water. The inclusion of instream fate processes is an advantage over Log Normal analysis, which cannot simulate instream fate and is limited to simulations for one effluent discharge. Another advantage of Monte Carlo is that model input data are not required to follow a specific statistical function, as in the Log Normal process. The Monte Carlo technique can also incorporate cross-correlation, and can estimate interaction of time varying parameters if the analysis is developed separately for each season and the results combined. Only Continuous Simulation can exactly calculate the effect of time varying parameters.

The primary disadvantage of Monte Carlo is the data requirement. Data on model input parameters are required to define the statistical distributions or the assumptions therein. Additional data are required for the calibration/verification of instream fate processes. However, in contrast to Continuous Simulation, the Monte Carlo Simulation can proceed and provide good results with a relatively sparse data set. Continuous Simulation requires a very complete data set. A secondary disadvantage to Monte Carlo is the inability to directly calculate running averages for results, as Continuous Simulation is able to do. Monte Carlo, like Log Normal, cannot directly calculate multiple day average instream concentrations but must estimate them by using multiple day averages to describe model inputs. A secondary disadvantage of the Monte Carlo technique is the large computational requirement. Like Continuous Simulation, however, the problem of excessive computer requirements is being minimized through recent advances in computer technology.

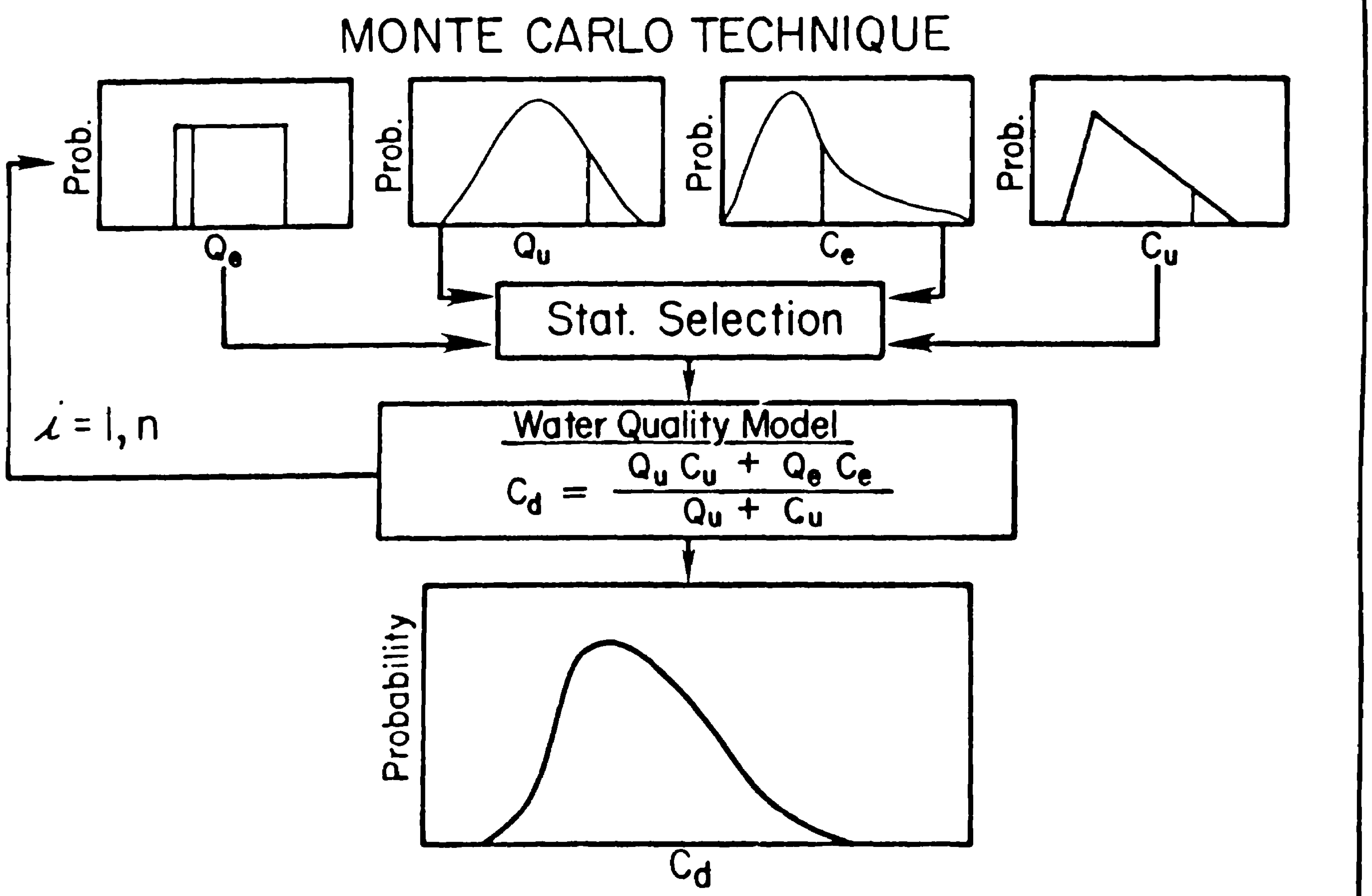

FIGURE 13

Schematic of Monte Carlo Technique

Input Requirements

The model input requirements for all three techniques were discussed in the Common Requirements chapter. This section details the specific input requirements for the Monte Carlo technique. These inputs are summarized in Table 2, and will be discussed in detail in this section. The inputs can be categorized into five groups:

- o general simulation requirements,
- o upstream data,
- o effluent data,
- o system physical and hydrological constraints, and
- o number of iterations.

General Simulation Requirements: The Monte Carlo method requires some general information on the system that will not change between simulations. The first basic input required for Monte Carlo is to establish the period of observed data to be used. This consists of the first year of observed data and the total number of years of data to use. The user should be cautious to select a period of duration for which a consistent data set is available. The user should not employ old data which are no longer representative of current conditions.

The second basic input required by Monte Carlo is the number of discharges in the system. The user must also determine if any of these discharges are located upstream of the USGS gaging station; if so, the average point source flow above the gage must be determined in order to correct the flow record. The final general input required is a computer file name to store these inputs. Once these general inputs are specified, they will be stored in this computer file and need not be specified for later simulations.

Upstream Boundary Data: The Monte Carlo technique requires statistical input distributions for the upstream boundary flow and concentration. The Monte Carlo technique allows the use of assumed data distributions or the observed data when selecting input distributions. The latter requires STORET data defining these conditions. STORET data defining boundary flow and concentration should be retrieved as described in the Data Requirements chapter, and stored in separate computer files.

DYNTOX currently allows four input distribution types to be used for Monte Carlo. The first three are standard statistical distributions: uniform (rectangular), normal (Gaussian), and triangular. The fourth distribution type, termed data-defined, is a non-standard statistical distribution. This choice can be used to simulate statistical distributions not currently supported by DYNTOX or in cases where the observed data follow no standard statistical distribution. The parameters required to describe these data should all be determined using SAS (UNIVARIATE procedure) and are described below. DYNTOX allows comparison of the observed data to the distribution selected by the user.

	Data Source
o General Information:	
- Beginning date of observed data	USGS flow records
- Number of years of observed data	USGS flow records
- Number of discharges above flow gage	User defined
- Average point source flow above gage	Treatment records
- TSS computer field name	User defined
o Upstream Data:	
- Flow Data	STORET
- Statistical Distribution for Flow	User defined
- Concentration Data	STORET
- Statistical Distribution for Concentration	User defined
o Effluent Data:	
- Flow data	Treatment records
- Statistical distribution for flow	User defined
- Concentration data	Treatment records
- Statistical distribution for concentration	User defined
o System Constants:	
- Time of travel information	Dye studies, current meters
- First order decay rate (s)	Instream data
- Drainage area ratio (s)	USGS topographic maps
- Water withdrawal rate (s)	Withdrawal records
o Number of Iterations	User defined

Table 2. Input Requirements for the Monte Carlo Technique

The uniform distribution represents the case where each value within a given range has an equal probability of occurrence. Two parameters are required to define a uniform distribution, the mean value and the range (See Figure 14).

The normal or Gaussian distribution is also shown in Figure 14. Two parameters are required to define this distribution, the mean value and standard deviation. The normal distribution is the only one that DYNTOX allows to have cross-correlation between parameters. If either effluent flow and concentration or boundary flow and concentration are specified as normal, the user may simulate cross-correlation between these parameters through the use of the bivariate normal distribution. The covariance between parameters is required if this option is selected, and can be determined using the COV option of the SAS procedures CORR or FUNCAT.

Triangular distributions are shown in Figure 14. The triangular distribution requires three parameters - the minimum value, expected value, and maximum value - and can therefore have a variety of different shapes.

Examples of the data defined distribution are shown in Figure 14. This distribution can take on an infinite number of shapes and can be used to simulate any desired distribution. The data defined distribution requires information on the minimum value, maximum value, and number of intervals to be used. For each interval, the user must specify the probability of occurrence for that range.

Effluent Data: Similar to upstream data, statistical distributions are needed in the model for effluent flow and concentration (or toxicity). For each effluent parameter, the user must specify a statistical distribution using the same technique described in the upstream boundary data section. Any downstream tributary input should be treated as a separate effluent input.

System Constants: System constants need to be defined for hydrologic and physical characteristics of the system. Program inputs for hydrologic data are needed to properly adjust gaged flow data to determine instream flow at different locations. Ratios are needed to define the comparison between the gauged drainage basin area and the drainage basin area at the point of discharge. These ratios adjust the USGS measured flows for nonpoint sources, and must be specified regardless of the location of the gaging station. For discharges located downstream of the USGS gage the ratio (and adjustment) will be greater than 1.0. For discharges located upstream of the gage, the ratio will be less than 1.0. The method to be used for specifying drainage area ratios is described in the Common Requirements chapter. A second hydrologic adjustment is required for water withdrawals. If a significant amount of water (>1% of river flow) is withdrawn from the river at any location, this withdrawal rate must be specified before performing a Monte Carlo waste load allocation.

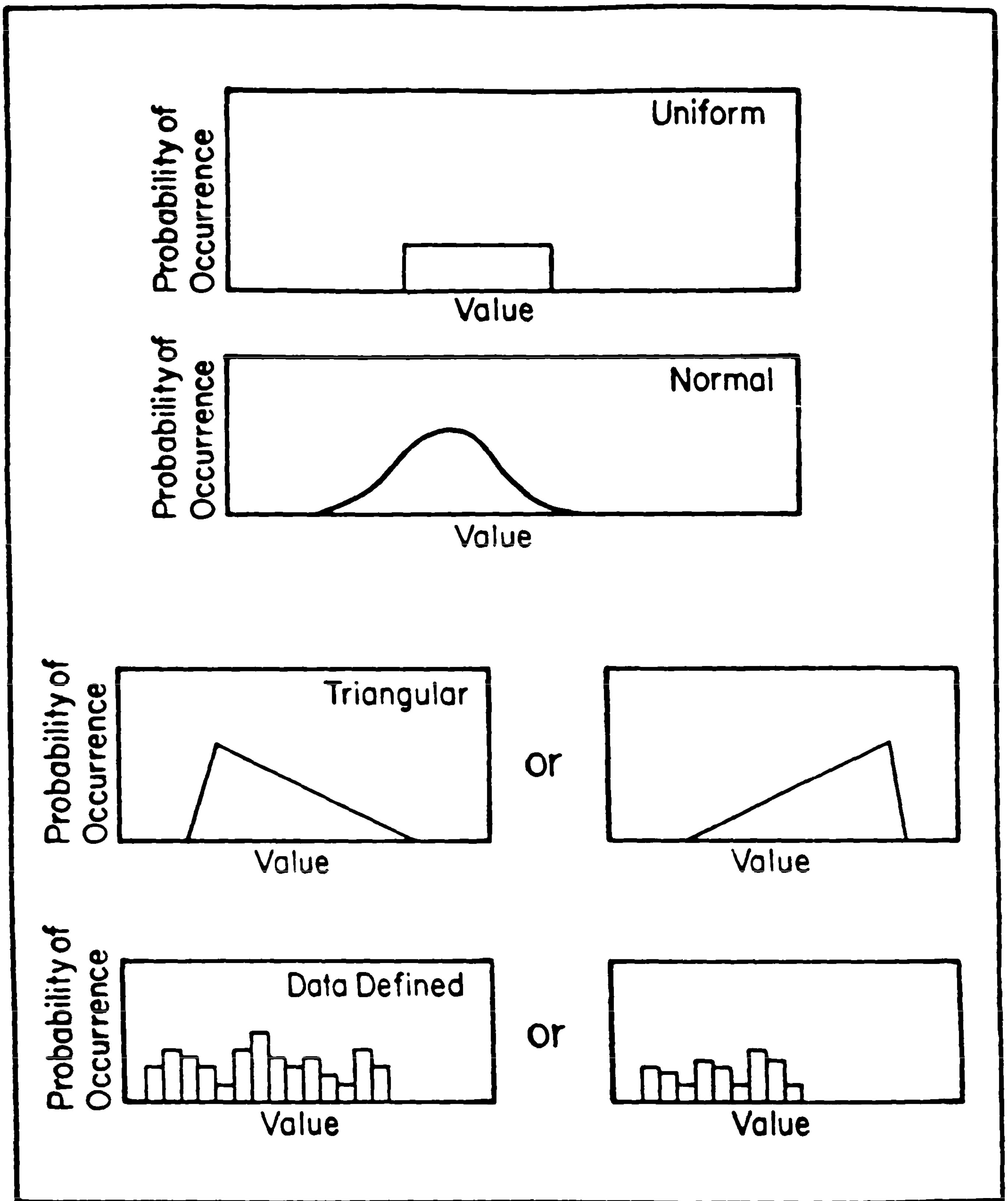

FIGURE 14

Example Monte Carlo Input Distributions

Another system constant required by Monte Carlo is the time-of-travel, which must be specified for the stream segment between the upstream boundary station and the first discharge and for the segments between each discharge. The method for specifying time of travel was discussed in detail in the Common Requirements chapter. Time of travel information need not be specified for the upstream segment in cases where the boundary station is located below a discharge as there is no upstream segment.

The first-order decay rate must be specified for each stream segment that requires time-of-travel information. The method for determining the first-order decay rate was discussed in the Data Requirements chapter.

Number of Iterations: The Monte Carlo technique requires a sufficient number of iterations to adequately define the probability of occurrence of downstream concentration. However, specifying too many iterations can waste computer time. The recommended method for determining the proper number of iterations is to run the Monte Carlo technique for an increasing number of iterations until the predicted probability distribution remains relatively constant. Five thousand (5000) iterations can be used as a starting point, with the number of iterations repetitively doubled until results remain constant. It is recommended that the three year return period value be compared when determining the proper number of iterations.

Program Use

The Monte Carlo program, like the programs for the other techniques, is divided into menu driven sub-programs (entitled activities) to allow the user as much flexibility as desired in performing simulations. The hierarchy of activities for Monte Carlo is shown in Figure 15. This section will describe how to use the Monte Carlo program and will discuss the options available to the user. It is divided into sections describing each of the primary activities:

- o Program Entry,
- o System Constants,
- o View Input Data/Specify Distributions,
- o Run Model,
- o View/Analyze Results, and
- o End Monte Carlo.

Program Entry: The first activity of the Monte Carlo technique is termed Program Entry. This section consists of specification of the time period of observed STORET data, number of discharges to be simulated, modeled point source flow above the USGS flow gage, and location of the data describing boundary conditions.

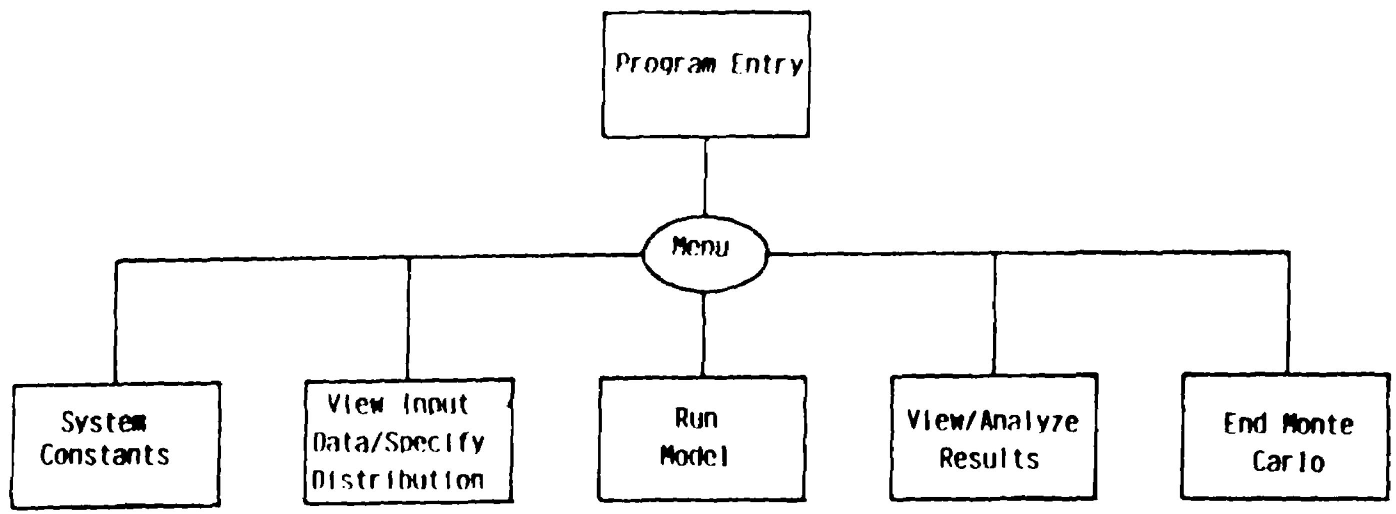

FIGURE 15

Hierarchy of Monte Carlo Subprograms

Figure 16 shows example sessions with the Program Entry activity. The first questions in Program Entry concern the existence and location of the TSS files for the simulation. TSS (Time Series Store) files are created by ANNIE to store time series information. The TSS file holds all information pertaining to the STORET boundary data for the Monte Carlo case. The first time a simulation is performed, the user should answer NO to the question asking if a TSS file was previously created, and specify a file name (Figure 16a). This will initiate the process to create a file. The user should answer YES to this question in subsequent simulations, and no other information will be required in the Program Entry section except the name of the TSS file (Figure 16b).

For first time entries, the TSS file name must be supplied. Any file name can be used that is compatible with the computer system. The next inputs required are the first year of observed data and the number of years of data. The required format for the date is Year/Month/Day (Figure 17a). Months and days with only one significant figure of information may be entered using only one digit. The next question in Program Entry before creation of the TSS file concerns the number of discharges in the system.

The TSS file for the system is being created and initialized at this point in Program Entry. This may take some time, depending on the computer system used, but the user will be informed when the file initialization is complete. TSS files created during Monte Carlo can be used for either of the other two DYNTOX techniques.

The final portion of Program Entry concerns defining the upstream boundary data files. Figure 16a shows an example session where both the boundary flow and boundary concentration data are located in STORET files. The user need only specify the name of the STORET data files and which data set of the STORET retrieval is to be used. The data set will always be one unless the user has multiple STORET retrievals stored in the same file. The section provides the ability to screen out flow and concentration data above acceptable values.

Another possibility for Program Entry is when the user has no STORET data and wishes to enter observed data manually from the terminal. Figure 16c shows an example of this situation. The user is required to input the number of data points, then the date and concentration for each value. The proper format for the data is (date, value) with the date in the YYMMDD format. The final option of program entry concerns the case where all input distributions were calculated off-line before using DYNTOX. In this case, no raw data need be entered, either from STORET files or from the terminal. Instead, the user enters only the previously calculated distribution information. (e.g. Figure 18a).

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16a. New TSS File

```
TOXIC SUBSTANCE WASTELOAD ALLOCATION MODELING

WHICH TECHNIQUE DO YOU WANT TO USE:

 (1) CONTINUOUS SIMULATION: DILUTION AND DECAY
 (2) MONTE CARLO: DILUTION AND DECAY
 (3) LOG-NORMAL: DILUTION ONLY
 (4) END TOXICS WLA, RETURN TO ANNIE MENU
ENTER SELECTION (1-4)
(Hit return for 4)
➤ 2
DO YOU HAVE UPSTREAM BOUNDARY DATA FOR ANALYSIS?
➤ YES
HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
➤ NO
WHAT IS THE NAME OF YOUR NEW TSS FILE?
➤ TESTFILE
HOW MANY YEARS OF DATA DO YOU HAVE?
(Hit return for 1)
➤ 6
ENTER STARTING DATE.
➤ 1960/1/1
HOW MANY OUTFALLS ARE THERE IN THE SYSTEM?
(Hit return for 1)
➤ 1
HOW MANY OUTFALLS LIE ABOVE THE FLOW GAGE?
(Hit return for 0)
➤ 0.
PLEASE WAIT WHILE YOUR TSS FILE IS INITIALIZED ...

INITIALIZATION OF YOUR TSS FILE IS NOW COMPLETE.

DO YOU HAVE A STORET FLOW DATA FILE?
➤ Y
WHAT IS THE NAME OF THE STORET FILE?
➤ STORET.FLO
USE WHICH DATA SET?
(Hit return for 1)
➤ 1
WHAT IS THE MAXIMUM ACCEPTABLE FLOW VALUE?
(Hit return for 0.)
➤ 4999.
  6245 POINTS READ
DO YOU HAVE A STORET DATA FILE FOR UPSTREAM CONCENTRATION?
➤ YES
WHAT IS THE NAME OF THE STORET FILE?
➤ STORET.CON
USE WHICH DATA SET?
(Hit return for 1)
➤ 1
WHAT IS THE MAXIMUM CONCENTRATION VALUE?
(hit return for 0.)
➤ 1.0
  1154 POINTS READ
```

FIGURE 16

Example Session with Monte Carlo Program Entry

16b. Existing TSS File

```
    HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
>   YES
    WHAT IS THE NAME OF YOUR TSS FILE?
>   EXAMPLE
```

16c. Terminal Entry of Data

```
    HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
>   NO
    WHAT IS THE NAME OF YOUR NEW TSS FILE?
>   TESTFILE
    HOW MANY YEARS OF DATA DO YOU HAVE?
    (Hit return for 1)
>   6
    HOW MANY OUTFALLS ARE THERE IN THE SYSTEM?
    (Hit return for 1)
>   1
    HOW MANY OUTFALLS LIE ABOVE THE FLOW GAGE?
    (Hit return for 0)
>   0

    PLEASE WAIT WHILE YOUR TSS FILE IS INITIALIZED ...

    INITIALIZATION OF YOUR TSS FILE IS NOW COMPLETE.

    DO YOU HAVE A STORET FLOW DATA FILE?
>   Y
    WHAT IS THE NAME OF THE STORET FILE?
>   STORET.FLO
    USE WHICH DATA SET?
    (Hit return for 1)
>   1
    WHAT IS THE MAXIMUM ACCEPTABLE FLOW VALUE?
    (Hit return for 0.)
    4999.
     6245 POINTS READ

    DO YOU HAVE A STORET DATA FILE FOR UPSTREAM CONCENTRATION?
>   NO
    DO YOU WANT TO ENTER CONCENTRATION DATA FROM THE TERMINAL?
>   YES
    HOW MANY SAMPLES DO YOU HAVE?
    (Hit return for 4)
>   3

    ENTER DATE AND UPSTREAM CONCENTRATION FOR EACH SAMPLE:
>   600101, .5
>   601231, .4
>   650615, .23
         3 POINTS READ
```

FIGURE 16 Cont'd.

Example Session with Monte Carlo Program Entry

```
MONTE CARLO SIMULATION TECHNIQUE: MAIN MENU

PLEASE SELECT ONE:

(1) SPECIFY SYSTEM CONSTANTS
(2) VIEW INPUT DATA/SPECIFY DISTRIBUTIONS
(3) RUN MODEL
(4) VIEW/ANALYZE RESULTS
(5) END MONTE CARLO SIMULATION, RETURN TO TOXICS WLA MENU
ENTER SELECTION (1-5)
(Hit return for 4)
1

SPECIFICATION OF SYSTEM CONSTANTS

HOW DO YOU WANT TO SPECIFY THE TIME OF TRAVEL RELATIONSHIP FROM
THE BOUNDARY TO THE FIRST DISCHARGE
(1) CONSTANT
(2) AS A FUNCTION OF FLOW
ENTER 1 OR 2
(hit return for 1)
1
WHAT IS THE TIME OF TRAVEL IN DAYS
(Hit return for 0.)
.1
WHAT IS THE FIRST ORDER DECAY RATE FROM
THE BOUNDARY TO THE FIRST DISCHARGE
USE UNITS OF (1/DAY)
(Hit return for 0.)
.1
WHAT IS THE WITHDRAWAL RATE
0.0
WHAT IS THE DRAINAGE AREA RATIO OF DISCHARGE # 1
TO THE USGS GAGE
(Hit return for 1.)
1.
```

FIGURE 17

Example Session with Monte Carlo System Constants

18a. Demonstration of Uniform and Normal Distributions

```
PLEASE CHOOSE ONE:

 (1) SPECIFY EFFLUENT FLOW/CONCENTRATION DISTRIBUTION
 (2) VIEW DATA/DETERMINE BOUNDARY CONCENTRATION DISTRIBUTION
 (3) VIEW DATA/DETERMINE BOUNDARY FLOW DISTRIBUTION
 (4) END INPUT DEFINITION, RETURN TO MONTE CARLO MENU

ENTER SELECTION (1-4)
(Hit return for 4)
➤ 1

 SPECIFICATION OF EFFLUENT DISTRIBUTIONS

SPECIFY FLOW INFORMATION FOR DISCHARGE   1
WHAT TYPE OF DISTRIBUTION DO YOU WANT?
 (1) UNIFORM
 (2) NORMAL
 (3) TRIANGULAR
 (4) DATA DEFINED
ENTER SELECTION (1-4)
(Hit return for 1)
➤ 1
WHAT IS THE MEAN VALUE
(Hit return for 1.)
➤ 25.
WHAT IS THE RANGE
(Hit return for 0.)
➤ 3.
SPECIFY CONCENTRATION INFORMATION FOR DISCHARGE   1
WHAT TYPE OF DISTRIBUTION DO YOU WANT?
 (1) UNIFORM
 (2) NORMAL
 (3) TRIANGULAR
 (4) DATA DEFINED
ENTER SELECTION (1-4)
(Hit return for 1)
➤ 2
WHAT IS THE MEAN VALUE
(Hit return for 1.)
➤ 5.
WHAT IS THE STANDARD DEVIATION
(Hit return for 0.)
➤ 1.

 END OF DISCHARGE SPECIFICATION SECTION
```

FIGURE 18

Example Session with Monte Carlo
Specifying Effluent Distributions

18b. Bivariate Normal Distribution

```
          SPECIFICATION OF EFFLUENT DISTRIBUTIONS

         SPECIFY FLOW INFORMATION FOR DISCHARGE   1
         WHAT TYPE OF DISTRIBUTION DO YOU WANT?
          (1) UNIFORM
          (2) NORMAL
          (3) TRIANGULAR
          (4) DATA DEFINED
         ENTER SELECTION (1-4)
         (Hit return for 1)
>        2
         WHAT IS THE MEAN VALUE
         (Hit return for 1.)
>        25.
         WHAT IS THE STANDARD DEVIATION
         (Hit return for 0.)
>        3.
         SPECIFY CONCENTRATION INFORMATION FOR DISCHARGE   1
         WHAT TYPE OF DISTRIBUTION DO YOU WANT?
          (1) UNIFORM
          (2) NORMAL
          (3) TRIANGULAR
          (4) DATA DEFINED
         ENTER SELECTION (1-4)
         (Hit return for 1)
>        2
         WHAT IS THE MEAN VALUE
         (Hit return for 1.)
>        5.
         WHAT IS THE STANDARD DEVIATION
         (Hit return for 0.)
>        1.
         IS CONCENTRATION CORRELATED TO FLOW
>        YES
         ENTER COVARIANCE BETWEEN CONCENTRATION AND FLOW
         (Hit return for 0.)
>        .2

          END OF DISCHARGE SPECIFICATION SECTION
```

FIGURE 18 Cont'd.

Example Session with Monte Carlo
Specifying Effluent Distributions

After completing Program Entry the program enters the main portion of Monte Carlo. The user will be given the menu shown in Figure 17 and must select one of the five activities:

1. System Constants
2. View Data/Specify Distributions
3. Run the Simulation
4. View/Analyze Model Results
5. End Simulation

Although there is flexibility in the order in which options are selected, system constants must be specified before choosing any other option (except ending).

System Constants: The system constants consist of time of travel, first-order decay rate, drainage area ratio, and water withdrawal rate. Program operation for the section is straightforward, requiring only the inputs discussed in the Common Requirements section. An example session specifying system constants is shown in Figure 17.

View Data/Specify Distributions: This section allows the user to view and/or analyze the observed data for the boundary parameters and then requires specification of the input distribution for these and the effluent parameters. Upon entry to the section, the user is given a menu (Figure 18) of four choices:

1) Specify effluent flow/concentration distribution,
2) View data/determine boundary concentration distribution,
3) View data/determine boundary flow distribution,
4) End input definition.

The options may be selected in any order desired; however, options 1-3 must be successfully completed before ending to successfully perform the model simulations.

Example sessions using the first option, specification of effluent data are shown in Figure 18. This session demonstrates use of the uniform and normal input distributions. A uniform distribution is selected for effluent flow in this example, and the user is required to supply a mean value and range (Figure 18a). A normal distribution is selected for effluent concentration; in this case, the user must supply a mean value and standard deviation. In the special case where normal distributions are selected for both flow and concentration, the option exists to specify a covariance term to represent the cross-correlation between parameters (Figure 18b). The same option exists when specifying normal distributions for boundary flow and boundary concentration.

When boundary concentration and flow data are available, the user has the option to view a plot of the actual data distribution or see a table describing the statistics and distribution of the data. Figure 19 shows an example session specifying boundary flow, where the user selects to see the plot of the data. The plot shows the probability of occurrence for the parameter over a number of ranges. The distribution is selected after viewing the data plot; in this case a triangular distribution. In cases where the data has been viewed or analyzed, the option exists to compare the predicted distribution to the observed data and also to determine its acceptability. The user is allowed to choose a new distribution for the parameter in cases where the fit is unacceptable.

Figure 20 shows an example session specifying boundary flow. This example demonstrates use of the data defined distribution. The sum of probabilities specified for all of the intervals in data defined must equal 1.0 or they will be rejected by the program and new values required.

In many cases, insufficient data will be available to define distribution for four-day average values. Based upon the Central Limit Theorem, users may specify a normal distribution for the parameter in question, with a standard deviation one half of that in the observed data as an estimate of the distribution of four day average value. The mean value will remain constant.

Running the Simulation: Only one input is required when choosing to run the simulation, the number of iterations. During the simulation, the program will print a message after the completion of every 2000 iterations to help in monitoring program progress.

View/Analyze Model Results: Model results can be seen in one of two formats, as a plot showing probability of exceedance for all concentrations, or as a statistics table showing statistics on the results along with the frequency distribution of the results in tabular format. An example session viewing the results of a model run in plot form is given in Figure 21. Figure 22 shows the results of the same simulation in tabular format. The statistics table consists of the statistical parameters mean, standard deviation, and coefficient of variation, along with the probability of occurrence for a number of intervals. The table also shows the probability of exceedance and the return period (recurrence interval) for a number of values. The option exists to view the return period for a value not shown if desired, or to view the value with a three year return period.

End the Simulation: Choosing this option allows the user to exit the Monte Carlo technique and return to the main DYNTOX menu. This option can be selected at any time during the Monte Carlo simulation.

```
SPECIFICATION OF INPUT DISTRIBUTIONS

OVER HOW MANY DAYS DO YOU WANT RESULTS AVERAGED
(Hit return for 1)
1
PLEASE CHOOSE ONE:

 (1) SPECIFY EFFLUENT FLOW/CONCENTRATION DISTRIBUTION
 (2) VIEW DATA/DETERMINE BOUNDARY CONCENTRATION DISTRIBUTION
 (3) VIEW DATA/DETERMINE BOUNDARY FLOW DISTRIBUTION
 (4) END INPUT DEFINITION, RETURN TO MONTE CARLO MENU

ENTER SELECTION (1-4)
(Hit return for 4)
3

 SPECIFICATION OF BOUNDARY FLOW DISTRIBUTION

DO YOU WANT TO SEE A DATA DISTRIBUTION PLOT BEFORE CHOOSING?
Y
INTERVAL OR CUMULATIVE FORMAT
I
DO YOU WANT TO SEE A STATISTICS TABLE?
N
WHAT TITLE DO YOU WANT FOR YOUR PLOT (80 CHARACTER MAXIMUM)
BOUNDARY FLOW
```

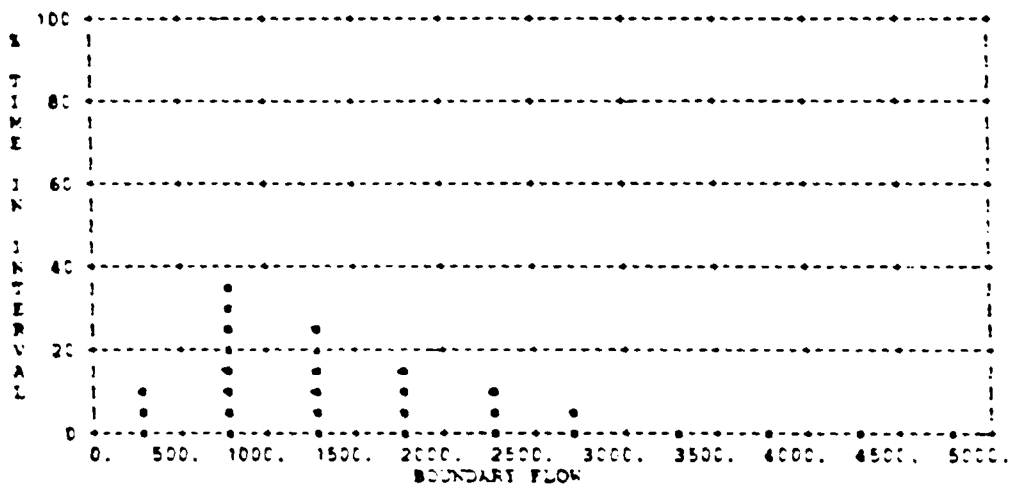
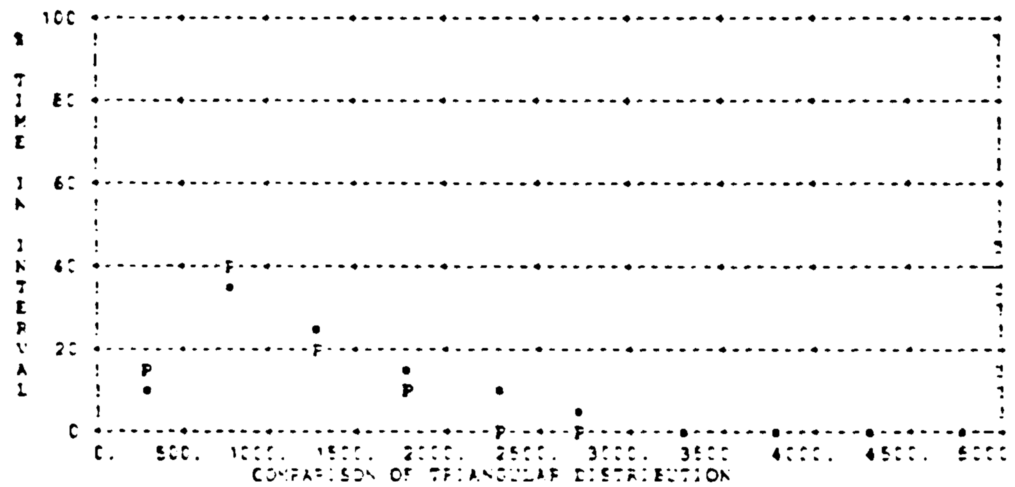


FIGURE 19

Example Session with Monte Carlo Specifying Triangular Distribution

```
SPECIFY BOUNDARY FLOW DISTRIBUTION
WHAT TYPE OF DISTRIBUTION DO YOU WANT?
 (1) UNIFORM
 (2) NORMAL
 (3) TRIANGULAR
 (4) DATA DEFINED
ENTER SELECTION (1-4)
(Hit return for 1)
3
WHAT IS THE MINIMUM VALUE
(Hit return for 0.)
10.
WHAT IS THE MAXIMUM VALUE
(Hit return for 1.)
2500.
WHAT IS THE EXPECTED VALUE
(Hit return for 0.5)
600.
DO YOU WANT TO COMPARE THE DISTRIBUTION TO THE ACTUAL DATA?
Y
WHAT TITLE DO YOU WANT FOR YOUR PLOT (80 CHARACTER MAXIMUM)
COMPARISON OF TRIANGULAR DISTRIBUTION
```




```
IF THIS FIT ACCEPTABLE?
Y
END OF BOUNDARY FLOW SPECIFICATION SECTION
```

FIGURE 19 Cont'd.

Example Session with Monte Carlo Specifying Triangular Distribution

```
SPECIFICATION OF BOUNDARY FLOW DISTRIBUTION


SPECIFY BOUNDARY FLOW DISTRIBUTION
WHAT TYPE OF DISTRIBUTION DO YOU WANT?
 (1) UNIFORM
 (2) NORMAL
 (3) TRIANGULAR
 (4) DATA DEFINED
ENTER SELECTION(1-4)
(Hit return for 1)
4
WHAT IS THE MINIMUM VALUE
(Hit return for 0.)
180.
HOW MANY INTERVALS DO YOU WANT TO SPECIFY
(Hit return for 2)
4
MINIMUM VALUE FOR INTERVAL 1 IS    180.
WHAT IS THE MAXIMUM VALUE
(Hit return for 1.)
220.
WHAT IS THE PROBABILITY OF OCCURRENCE
(Hit return for 0.)
.66667
MINIMUM VALUE FOR INTERVAL 2 IS    220.
WHAT IS THE MAXIMUM VALUE
(Hit return for 220.)
260.
WHAT IS THE PROBABILITY OF OCCURRENCE
(Hit return for 0.)
0.
MINIMUM VALUE FOR INTERVAL 3 IS    260.
WHAT IS THE MAXIMUM VALUE
(Hit return for 260.)
320.
WHAT IS THE PROBABILITY OF OCCURRENCE
(Hit return for 0.)
0.
MINIMUM VALUE FOR INTERVAL 4 IS    320.
WHAT IS THE MAXIMUM VALUE
(Hit return for 320.)
340.
WHAT IS THE PROBABILITY OF OCCURRENCE
(Hit return for 0.)
.33333
DO YOU WANT TO COMPARE THE DISTRIBUTION TO THE ACTUAL DATA
NO

END OF BOUNDARY FLOW SPECIFICATION SECTION
```

FIGURE 20

Example Session Specifying Data Defined Distribution

```
MONTE CARLO TECHNIQUE

   PLEASE CHOOSE FROM THE FOLLOWING:

   (1) SPECIFY SYSTEM CONSTANTS
   (2) RUN MODEL
   (3) VIEW/ANALYZE RESULTS
   (4) END MONTE CARLO SIMULATION, RETURN TO TOXICS WLA MENU

   ENTER YOUR CHOICE (1 - 4):
(Hit return for 1)
3

VIEWING ANALYSIS OF RESULTS

DO YOU WANT TO SEE A PLOT?
Y
WHAT TITLE DO YOU WANT FOR YOUR PLOT (80 CHARACTER MAXIMUM)
MONTE CARLO CONCENTRATION
```

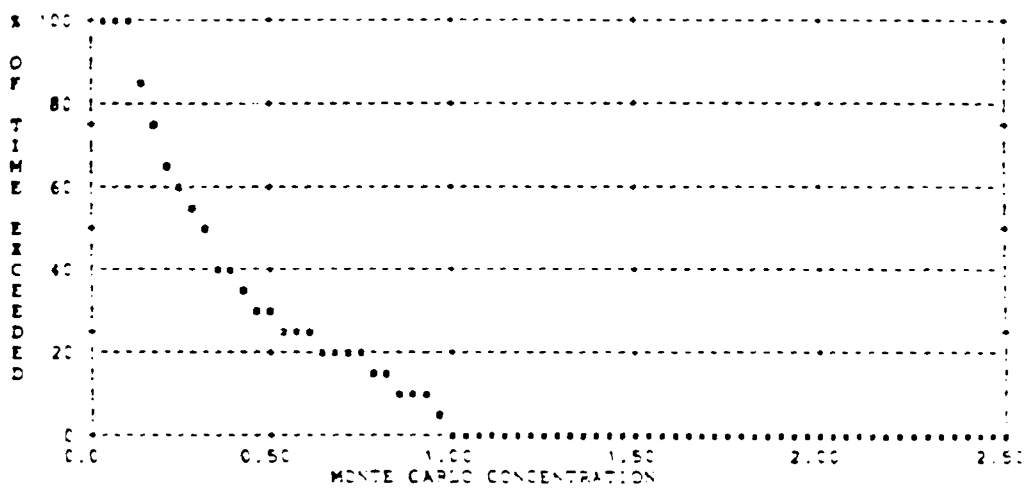


FIGURE 21

Example Session with Monte Carlo Viewing Results in Plot Format

```
   PLEASE CHOOSE FROM THE FOLLOWING:

   (1) SPECIFY SYSTEM CONSTANTS
   (2) RUN MODEL
   (3) VIEW/ANALYZE RESULTS
   (4) END CONTINUOUS SIMULATION
   ENTER YOUR CHOICE (1 - 4):
(Hit return for 1)
3

VIEWING/ANALYSIS OF RESULTS

DO YOU WANT TO SEE A PLOT?
N
DO YOU WANT TO SEE A STATISTICS TABLE?
Y

WHAT TITLE DO YOU WANT FOR YOUR TABLE (80 CHARACTER MAXIMUM)
MONTE CARLO

                                MONTE CARLO

     MEAN =        0.404       STANDARD DEVIATION =       0.280
     COEFFICIENT OF VARIATION =        0.693

---------------------------------------------------------------------------
 VALUE     % OF TIME EXCEEDED  % OF TIME IN INTERVAL  RETURN PERIOD (YEARS)
---------------------------------------------------------------------------

 0.0          100.000                                      0.003
                                   40.244
 0.250         59.756                                      0.005
                                   30.081
 0.500         29.675                                      0.009
                                   11.382
 0.750         18.293                                      0.015
                                   16.260
  1.00          2.033                                      0.135
                                    2.033
  1.25          0.0                                     -999.000
                                    0.0
  1.50          0.0                                     -999.000
                                    0.0
  1.75          0.0                                     -999.000
                                    0.0
  2.00          0.0                                     -999.000
                                    0.0
  2.25          0.0                                     -999.000
                                    0.0
  2.50          0.0                                     -999.000
---------------------------------------------------------------------------

DO YOU WANT TO: (1) SEE A RETURN PERIOD FOR A DIFFERENT VALUE
     (2) CALCULATE THE VALUE WITH A THREE YEAR RETURN PERIOD
 OR  (3) END TABULAR ANALYSIS
3
```

FIGURE 22

Example Session with Monte Carlo Viewing Results in Tabular Format

V. LOG NORMAL

The third technique that can be used to calculate a probability distribution for instream toxics concentrations is Log Normal probabilistic analysis. This technique assumes that all input parameters can be described by a log normal statistical distribution, and uses numerical integration to predict the concentration distribution below a single effluent discharge. The Log Normal technique has many advantages as it:

- predicts frequency and duration of concentrations:
- requires less computational expense than Continuous Simulation or Monte Carlo;
- does not require extensive time-series data as Continuous Simulation;
- incorporates cross-correlation of parameters.

The primary disadvantages to Log Normal are that extensive data are required to define input distributions, all parameters are assumed to be log normally distributed, and instream losses or simulation of more than one discharge cannot be considered.

This chapter describes the theory and application of the Log Normal technique, and is divided into three sections. The first section discusses the theory upon which the Log Normal technique is based, and its advantages and disadvantages. The second section describes the data input requirements. The third and final section details how to use the computer program of the Log Normal technique when performing waste load allocations.

Theory

Continuous Simulation and Monte Carlo and Log Normal analysis are based upon the same dilution equation, which predicts the concentration below a discharge (C_d) based upon upstream concentration (C_u), upstream flow (Q_u) effluent concentration (C_e), and effluent flow (Q_e):

$$C_d = \frac{Q_u C_u + Q_e C_e}{Q_u + Q_e} \qquad (4)$$

This equation is suitable for all in-stream modeling except mixing zone analysis. Where Continuous Simulation and Monte Carlo analysis solve this equation many thousands of times using different values for the inputs, Log Normal analysis uses a totally different technique.

Log Normal analysis requires that each model input follow a log normal statistical distribution; this causes the probability distribution for each equation to be well defined mathematically. The probability that the downstream river concentration (C_d) exceeds any given value, C^*, can be expressed as a multiple integral of the joint probability density functions over the values of flows and concentrations for which $C_d > C$. Since the variation of each input variable is defined by a mathematical equation, numerical integration can be conducted to determine the probability that $C_d > C$. By repeating this integration for different values of C, the probability distribution for C_d can be estimated. The probability of exceedance can be estimated for durations other than one day by using inputs representative of multiple-day averages. For a more complete description of the theory behind Log Normal probabilistic analysis, see DiToro (1984).

The primary advantage of the Log Normal technique is the ability to predict the frequency distribution of the river concentration without the excessive computational requirements of Continuous Simulation or Monte Carlo. Whereas Continuous Simulation and Monte Carlo require several thousand iterations of the model to predict the concentration distribution, Log Normal can proceed much faster through numerical integration.

The disadvantages of Log Normal are the inability to simulate multiple discharge situations and the requirement that all parameters follow log normal distributions. In many cases, parameter data only approximately conform to a log normal distribution. This introduces errors which are exagerated at the infrequent recurrence levels of the probablistic simulation. Log Normal also has the same disadvantage as Monte Carlo in that multiple day average in-stream concentrations can only be approximated through the use of averaged inputs. Continuous Simulation is the only technique that allows exact determination of multiple day average results. Log Normal analysis also requires significantly more input data thar steady state models, but no more than Continuous Simulation or Monte Carlo.

Input Requirements

The model input requirements for all three techniques were discussed in the Data Requirements chapter. This section details the specific input requirements for the Log Normal technique. These inputs are summarized in Table 3, and will be discussed in detail in this section. The inputs can be categorized into five groups: general simulation requirements, upstream data, effluent data, system hydrological constraints, and output range of interest. However, the data requirements for each are to an extent first dictated by general information on the simulation.

General Simulation Requirements: Log Normal analysis requires some general information on the system that will not change between simulations. The first basic input required for Log Normal Analysis is to establish the period of observed data to be used. This consists of the first year of observed data and the total number of years of data to use. The user should be cautious to select a period of duration for which a complete and consistent data set is available. Caution should be directed towards using old data which are no longer representative of current conditions.

The second basic input required by Log Normal is whether the discharge is located upstream of the USGS gaging station. If so, the average point source flow above the gage must be determined. The final general input required is a computer file name to store these inputs. Once these general inputs are specified, they will be stored in this computer file and need not be specified for later simulations.

	Data Source
o General Information:	
- Beginning date of observed data	USGS flow records
- No. of years of observed data	USGS flow records
- Number of discharges above flow gage	User defined
- Average point source flow above gage	Treatment records
- TSS computer file name	User defined
o Upstream Data:	
- Mean and 84th percentile value for flow	STORET
- Cross-correlation between river flow and river concentration	SAS
- Mean and 84th percentile value for concentration	STORET
- Cross-correlation between river flow and effluent flow	SAS
o Effluent Data:	
- Mean and 84th percentile value for flow	STORET
- Mean and 84th percentile value for concentration	STORET
- Cross-correlatiion between effluent flow and effluent concentration	
o System Constants:	
- Drainage area ratio	USGS topographic maps
- Water withdrawal rate	Withdrawal records
o Output Interval of Interest:	
- Minimum river concentration of interest	User defined
- Maximum river concentration of interest	User defined
- Interval for output	User defined

Table 3. Input Requirements for the Log Normal Technique

Upstream Boundary Data: The Log Normal technique requires the mean and variance of the input distributions for the upstream boundary flow and concentration. DYNTOX provides the ability to determine the distribution parameters from observed upstream boundary flow and concentration. This requires STORET data defining these conditions.

The required form of this data includes the 50th percentile (mean) value and 84th percentile value for each parameter. These parameters can also be determined from SAS, as well as the adequacy of the assumption of log normality (using the UNIVARIATE procedure on the logarthims of the observed data). Boundary flow data must be corrected for point source flows and withdrawals before performing SAS analysis, as they may significantly affect the assumption of log normality. In addition, this technique requires information describing the cross-correlation between river flow and effluent flow, and river flow and river concentration. These cross-correlations can also be determined using SAS, using the CORR procedure.

Effluent Data: Similar to upstream data, log normal distribution parameters are needed in the model for effluent flow and concentration (or toxicity). For each effluent parameter, the user must specify a mean and 84th percentile using the same technique described in the upstream boundary data section. DYNTOX does not provide the capability to calculate these values directly from observed effluent data. However, SAS may be used to calculate these parameters before performing Log Normal analysis. The final effluent requirement is the cross-correlation between effluent flow and concentration. This may also be determined through SAS.

System Constants: Program inputs for hydrologic data are needed to properly adjust gaged flow data to determine instream flow at different locations. Ratios are needed to define the comparison between the gauged drainage basin area and the drainage basin area at the point of discharge. This ratio adjusts the USGS measured flows for nonpoint sources, and must be specified regardless of the location of the gaging station. For a discharge located downstream of the USGS gage the ratio (and adjustment) will be greater than 1.0. For a discharge located upstream of the gage, the ratio will be less than 1.0. The method to be used for specifying drainage area ratios is described in the Data Requirements chapter. A second hydrologic adjustment is required for water withdrawals. If a significant amount of water (>1% of river flow) is withdrawn from the river at any location between the gage and the outfall, this withdrawal rate must be specified before performing a waste load allocation.

Output Range of Interest: The user must specify the minimum and maximum output concentration of interest and desired output interval before running the simulation, due to the nature of the solution technique. Care should be taken to choose a minimum value that has a non-zero probability of exceedance. Minimum values that have an insignificant probability of exceedance will be rejected by the program, and replacement values will be required.

Program Use

The Log Normal program, like the programs for the other techniques, is divided into menu-driven subprograms (entitled activities) to allow as much flexibility as possible in performing the simulation. The hierarchy of activities for Log Normal analysis is shown in Figure 23. This section will describe how to use the Log Normal program and will discuss the options available. It is divided into sections describing each of the primary activities of Log Normal analysis: Program Entry, Input Specification, Model Simulation, Statistical Analysis of Inputs/Results, Plots of Inputs/Results.

Program Entry: The first activity of the Log Normal technique is termed Program Entry. This section consists of specification of the time period of observed STORET data, modeled point source flow above the USGS flow gage, location of the data describing boundary conditions, and withdrawals between the USGS gage and the effluent outfall.

Figure 24 shows example sessions with the Program Entry activity. The first questions in Program Entry concern the existence and location of the TSS files for the simulation. TSS (Time Series Store) files are created by ANNIE to store time series information. For the Log Normal technique, the TSS file holds all information pertaining to the STORET boundary data. The user should answer NO to the question asking if a TSS file was previously created the first time a simulation is performed, and specify a TSS file name (Figure 24a). This will initiate the process to create a file. The user should answer YES to this question in subsequent simulations, and no other information will be required in the Program Entry section except the name of the TSS file (Figure 24b). A TSS file created for Log Normal analysis can also be used for Continuous Simulation or Monte Carlo.

For first-time entries, the TSS file name must be supplied. Any file name compatible with the computer system in use is acceptable. The next inputs required of the user are the first year of observed data and the number of years of data that exist. The required format for the date is Year/Month/Day (Figure 24a). Months and days with only one significant figure of information may be entered using only one digit. At this point in Program Entry, the TSS file for the system is being created and initialized. This may take some time, depending on the computer system used, but the user will be informed when the initialization is complete.

The final portion of the Program Entry concerns location of the STORET data. Figure 24a shows an example session where both the boundary flow and boundary concentration data are located in STORET files. The user need only specify the name of the STORET data files and which data set of the STORET retrieval is to be used. The program provides the capability to screen out flow and concentration data above acceptable values.

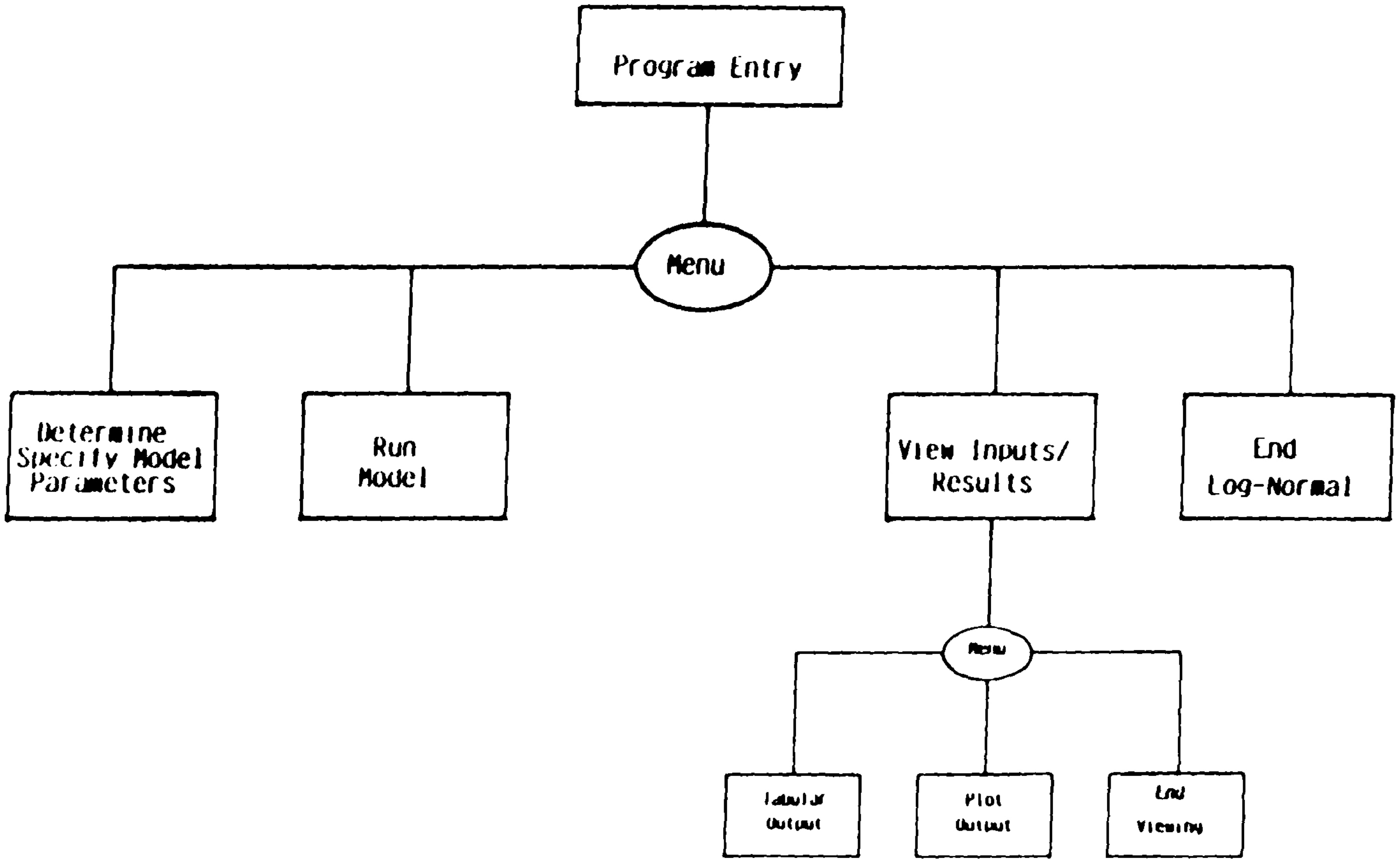


FIGURE 23

Hierarchy of Subprograms for Log Normal

Another possibility for Program Entry is when the user has no STORET data and wishes to enter data manually from the terminal (Figure 24c). The user is required to input the number of data points, then the date and concentration for each value. The proper format for the data is (date, value) with the date in the YYMMDD format. The final option of the Program Entry concerns the case where all input distributions were calculated off-line before using the DYNTOX. In this case, no data need be entered, either from STORET files or from the terminal, and the user may proceed directly to Input Specification.

Input Specification: Required inputs include mean (50th percentile) and 84th percentile values for all model parameters, along with the cross-correlation between river flow and effluent flow, between river flow and river concentration, and between effluent flow and effluent concentration. Values for the 50th and 84th percentile values for the boundary parameters will be calculated from the observed data when available. An example session demonstrating Log Normal Input Specification is shown in Figure 25.

In many cases, insufficient data will be available to define distribution for four-day average values. In these situations, users may specify a log normal distribution for the parameter in question, with a standard deviation one half of that in the observed data as an estimate of the distribution of four day average values.

Model Simulation: Model simulation requires the specification of a minimum and maximum value of interest and the interval that results are desired. It is important to note that this interval is in log (base 10) units. When conducting wasteload allocations, the user should select the minimum, maximum, and increment value such that the return period for the water quality criterion will be output. One way to assure this occurrence is to specify the minimum and/or maximum value to be the criteria. An example session showing model simulation is given in Figure 26.

Statistical Analysis of Inputs/Results: The user has the ability to view any of the model input parameters or the simulation results in tabular format, receiving statistical results and a table of the frequency distribution. This section can be assessed any time after the simulation has been run. After specifying the parameter to be viewed and a one-line 80 character maximum title, results shown in Figure 27 demonstrate this feature using model results. The output for model input parameters has an identical format.

Plots of Inputs/Results: The user also has the ability to view any of the model input parameters frequency distribution in plot form. The plot format differs slightly between the input parameters and model results. The input parameters are plotted as the probability of occurrence over a number of ranges (see Figure 28). The model results are plotted as the overall probability of exceedance for each value in the specified range (Figure 29).

24a. New TSS File

```
        TOXIC SUBSTANCE WASTELOAD ALLOCATION MODELING

        WHICH TECHNIQUE DO YOU WANT TO USE:

         (1) CONTINUOUS SIMULATION: DILUTION AND DECAY
         (2) MONTE CARLO: DILUTION AND DECAY
         (3) LOG-NORMAL: DILUTION ONLY
         (4) END TOXICS WLA, RETURN TO ANNIE MENU
        ENTER SELECTION (1-4)
        (Hit return for 4)
      ➤ 3
        DO YOU HAVE UPSTREAM BOUNDARY DATA FOR ANALYSIS?
      ➤ YES
        HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
      ➤ NO
        WHAT IS THE NAME OF YOUR NEW TSS FILE?
      ➤ TESTFILE
        HOW MANY YEARS OF DATA DO YOU HAVE?
        (Hit return for 1)
      ➤ 6
        ENTER STARTING DATE.
      ➤ 1960/1/1
        HOW MANY OUTFALLS ARE THERE IN THE SYSTEM?
        (Hit return for 1)
      ➤ 1
        HOW MANY OUTFALLS LIE ABOVE THE FLOW GAGE?
        (Hit return for 0)
      ➤ 0.
        PLEASE WAIT WHILE YOUR TSS FILE IS INITIALIZED ...

        INITIALIZATION OF YOUR TSS FILE IS NOW COMPLETE.

        DO YOU HAVE A STORET FLOW DATA FILE?
      ➤ Y
        WHAT IS THE NAME OF THE STORET FILE?
        STORET.FLO
        USE WHICH DATA SET?
        (Hit return for 1)
      ➤ 1
        WHAT IS THE MAXIMUM ACCEPTABLE FLOW VALUE?
        (Hit return for 0.)
      ➤ 9999.
         6245 POINTS READ
        DO YOU HAVE A STORET DATA FILE FOR UPSTREAM CONCENTRATION?
      ➤ YES
        WHAT IS THE NAME OF THE STORET FILE?
      ➤ STORET.CON
        USE WHICH DATA SET?
        (Hit return for 1)
      ➤ 1
        WHAT IS THE MAXIMUM CONCENTRATION VALUE?
        (Hit return for 0.)
      ➤ 1.0
         1154 POINTS READ
```

FIGURE 24

Example Sessions with Log Normal Program Entry

24b. Existing TSS File

```
  HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
➤ YES
  WHAT IS THE NAME OF YOUR TSS FILE?
➤ EXAMPLE
```

24c. Terminal Entry of Data

```
  HAVE YOU PREVIOUSLY CREATED A TSS FILE FOR THIS SIMULATION?
➤ NO
  WHAT IS THE NAME OF YOUR NEW TSS FILE?
➤ TESTFILE
  HOW MANY YEARS OF DATA DO YOU HAVE?
  (Hit return for 1)
➤ 6
  ENTER STARTING DATE.
➤ 1960/1/1
  HOW MANY OUTFALLS ARE THERE IN THE SYSTEM?
  (Hit return for 1)
➤ 1
  HOW MANY OUTFALLS LIE ABOVE THE FLOW GAGE?
  (Hit return for 0)
➤ 0

  PLEASE WAIT WHILE YOUR TSS FILE IS INITIALIZED ...

  INITIALIZATION OF YOUR TSS FILE IS NOW COMPLETE.

  DO YOU HAVE A STORET FLOW DATA FILE?
➤ Y
  WHAT IS THE NAME OF THE STORET FILE?
➤ STORET.FLO
  USE WHICH DATA SET?
  (Hit return for 1)
➤ 1
  WHAT IS THE MAXIMUM ACCEPTABLE FLOW VALUE?
  (Hit return for 0.)
➤ 6999.
   6265 POINTS READ

  DO YOU HAVE A STORET DATA FILE FOR UPSTREAM CONCENTRATION?
➤ NO
  DO YOU WANT TO ENTER CONCENTRATION DATA FROM THE TERMINAL?
➤ YES
  HOW MANY SAMPLES DO YOU HAVE?
  (Hit return for 6)
➤ 3

  ENTER DATE AND UPSTREAM CONCENTRATION FOR EACH SAMPLE:
➤ 600101, .5
➤ 601231, .4
➤ 650615, .23
      3 POINTS READ
```

FIGURE 24 Cont'd.

Example Sessions with Log Normal Program Entry

```
LOGNORMAL SIMULATION TECHNIQUE

PLEASE SELECT ONE:

 (1) DETERMINE/SPECIFY MODEL PARAMETERS
 (2) RUN MODEL
 (3) VIEW MODEL RESULTS/INPUT DISTRIBUTIONS
 (4) END LOGNORMAL, RETURN TO TOXICS WLA MENU

ENTER SELECTION (1-4)
(Hit return for 4)
>
 (1) DETERMINE/SPECIFY MODEL PARAMETERS
 (2) RUN MODEL
 (3) VIEW MODEL RESULTS/INPUT DISTRIBUTIONS
 (4) END LOGNORMAL, RETURN TO TOXICS WLA MENU

ENTER SELECTION (1-4)
(Hit return for 4)
> 1
PARAMETER SPECIFICATION SECTION

OVER HOW MANY DAYS DO YOU WANT RESULTS AVERAGED
(Hit return for 1)
> 1
WHAT IS THE MEDIAN BOUNDARY FLOW
(Hit return for 1.)
> 1000.
WHAT IS THE 84% BOUNDARY FLOW
(Hit return for 10.)
> 10000.
WHAT IS THE CROSS-CORRELATION BETWEEN RIVER FLOW AND EFFLUENT
FLOW
(Hit return for 0.)
> .1
WHAT IS THE MEDIAN BOUNDARY CONCENTRATION
(Hit return for 1.)
> .1
WHAT IS THE 84% BOUNDARY CONCENTRATION
(Hit return for 10.)
> .5
WHAT IS THE CROSS-CORRELATION BETWEEN RIVER CONCENTRATION
RIVER FLOW
(Hit return for 0.)
> .1
```

FIGURE 25

Example Session with Log Normal Input Specification

```
    EFFLUENT FLOW SPECIFICATION

    WHAT IS THE MEDIAN EFFLUENT FLOW
    (Hit return for 1.)
➤   10.
    WHAT IS THE 84% EFFLUENT FLOW
    (Hit return for 10.)
➤   100.
    WHAT IS THE CROSS-CORRELATION BETWEEN EFFLUENT FLOW AND
    EFFLUENT CONCENTRATION
    (Hit return for 0.)
➤   .1
    EFFLUENT CONCENTRATION SPECIFICATION

    WHAT IS THE MEDIAN EFFLUENT CONCENTRATION
    (Hit return for 1.)
➤   10.
    WHAT IS THE 84% EFFLUENT CONCENTRATION
    (Hit return for 10.)
➤   100.
```

FIGURE 25 Cont'd.

Example Session with Log Normal Input Specification

```
LOGNORMAL SIMULATION TECHNIQUE

PLEASE SELECT ONE:

 (1) DETERMINE/SPECIFY MODEL PARAMETERS
 (2) RUN MODEL
 (3) VIEW MODEL RESULTS/INPUT DISTRIBUTIONS
 (4) END LOGNORMAL, RETURN TO TOXICS WLA MENU

ENTER SELECTION (1-4)
(Hit return for 4)
➤ 2
WHAT IS THE MINIMUM VALUE OF INTEREST
(Hit return fo. 0.)
➤ .01
WHAT IS THE MAXIMUM VALUE OF INTEREST
(Hit return for 0.)
➤ 100.
AT WHAT INCREMENT DO YOU WANT RESULTS LISTED (NOTE: THIS
INCREMENT MUST BE IN LOG UNITS!)
(Hit return for 0.)
➤ .5

SIMULATION COMPLETE
```

FIGURE 26

Example Session Performing Log Normal Simulation

```
LOGNORMAL SIMULATION TECHNIQUE

PLEASE SELECT ONE:

 (1) DETERMINE/SPECIFY MODEL PARAMETERS
 (2) RUN MODEL
 (3) VIEW MODEL RESULTS/INPUT DISTRIBUTIONS
 (4) END LOGNORMAL, RETURN TO TOXICS WLA MENU
ENTER SELECTION (1-4)
(Hit return for 4)
3
VIEW RESULTS/INPUTS FOR LOGNORMAL ANALYSIS

DO YOU WANT (1) PLOT OF FREQUENCY DISTRIBUTION
            (2) TABULAR OUTPUT
        OR  (3) END VIEWING, RETURN TO MAIN LOGNORMAL MENU
ENTER SELECTION (1-3)
(Hit return for 3)
WHAT DO YOU WANT TO SEE
    MODEL RESULTS:
(1) RIVER CONCENTRATION
    INPUT DISTRIBUTIONS:
(2) UPSTREAM FLOW
(3) UPSTREAM CONCENTRATION
(4) EFFLUENT FLOW
(5) EFFLUENT CONCENTRATION
ENTER SELECTION ( 1-5 )
(Hit return for 1)
1
WHAT TITLE DO YOU WANT (80 CHARACTERS MAXIMUM)
LOG-NORMAL RESULTS

                          LOG-NORMAL RESULTS

-----------------------------------------------------------------------------

 VALUE      % OF TIME EXCEEDED  % OF TIME IN INTERVAL  RETURN PERIOD (YEARS)

-----------------------------------------------------------------------------
0.100E-01        98.670                                      0.003
                                      5.410
0.316E-01        93.260                                      0.003
                                     14.429
0.100E+00        78.831                                      0.003
                                     22.649
0.316E+00        56.182                                      0.005
                                     22.000
0.100E+01        34.182                                      0.008
                                     15.071
0.316E+01        19.111                                      0.014
                                      8.860
0.100E+02        10.251                                      0.027
                                      5.166
0.316E+02         5.086                                      0.054
                                      2.876
0.100E+03         2.206                                      0.124
-----------------------------------------------------------------------------
```

FIGURE 27

Example Session with Tabular Output from Log Normal

```
LOGNORMAL SIMULATION TECHNIQUE

PLEASE SELECT ONE:

 (1) DETERMINE/SPECIFY MODEL PARAMETERS
 (2) RUN MODEL
 (3) VIEW MODEL RESULTS/INPUT DISTRIBUTIONS
 (4) END LOGNORMAL, RETURN TO TOXICS WLA MENU
ENTER SELECTION (1-4)
(Hit return for 4)
3
VIEW RESULTS/INPUTS FOR LOGNORMAL ANALYSIS

DO YOU WANT (1) PLOT OF FREQUENCY DISTRIBUTION
            (2) TABULAR OUTPUT
         OR (3) END VIEWING, RETURN TO MAIN LOGNORMAL MENU
ENTER SELECTION (1-3)
(Hit return for 3)
1
WHAT DO YOU WANT TO SEE
    MODEL RESULTS:
(1) RIVER CONCENTRATION
    INPUT DISTRIBUTIONS:
(2) UPSTREAM FLOW
(3) UPSTREAM CONCENTRATION
(4) EFFLUENT FLOW
(5) EFFLUENT CONCENTRATION
ENTER SELECTION ( 1-5 )
(Hit return for 1)
2
PLEASE ENTER THE TITLE OF THE PLOT (80 CHARACTERS MAXIMUM)
UPSTREAM FLOW
```

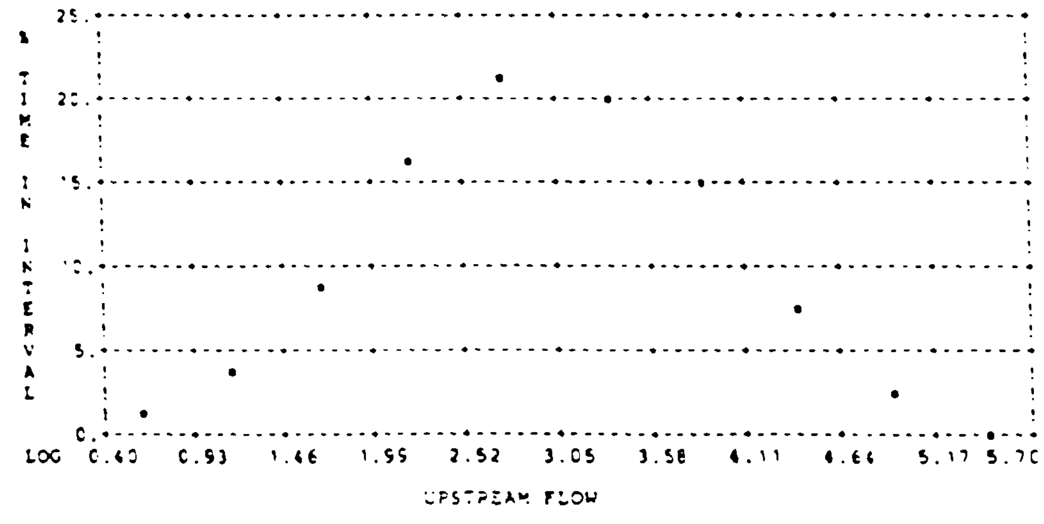


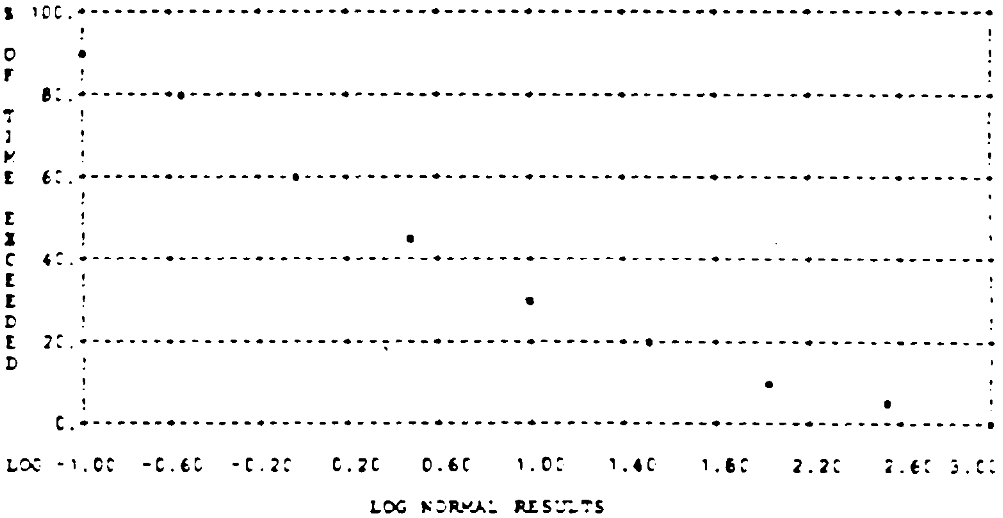
FIGURE 28

Example Session with Plot of Log Normal Inputs

```
VIEW RESULTS/INPUTS FOR LOGNORMAL ANALYSIS

DO YOU WANT (1) PLOT OF FREQUENCY DISTRIBUTION
            (2) TABULAR OUTPUT
         OR (3) END VIEWING, RETURN TO MAIN LOGNORMAL MENU

ENTER SELECTION (1-3)
(hit return for 3)
1
WHAT DO YOU WANT TO SEE
    MODEL RESULTS:
(1) RIVER CONCENTRATION
    INPUT DISTRIBUTIONS:
(2) UPSTREAM FLOW
(3) UPSTREAM CONCENTRATION
(4) EFFLUENT FLOW
(5) EFFLUENT CONCENTRATION
ENTER SELECTION ( 1-5 )
(Hit return for 1)
1
PLEASE ENTER THE TITLE OF THE PLOT (80 CHARACTERS MAXIMUM)
LOG NORMAL RESULTS
```




```
VIEW RESULTS/INPUTS FOR LOGNORMAL ANALYSIS

DO YOU WANT (1) PLOT OF FREQUENCY DISTRIBUTION
            (2) TABULAR OUTPUT
         OR (3) END VIEWING, RETURN TO MAIN LOGNORMAL MENU

ENTER SELECTION (1-3)
(Hit return for 3)
3
```

FIGURE 29

Example Session with Plot of Log Normal Results

VI. PERFORMING WASTE LOAD ALLOCATIONS

Overview

Each of the three techniques documented herein - Continuous Simulation, Monte Carlo, and Log Normal - can potentially be used to perform toxics waste load allocations. However, not all techniques can be applied in all situations. In general, Continuous Simulation should be used in cases where time series information on model inputs is well defined. Log Normal should be used in single discharge cases where all model parameters are approximately log normally distributed. Monte Carlo should be used when neither of the other techniques are applicable, or in conjunction with the other techniques. In some cases, the data may be insufficient to use any of the three techniques.

This chapter discusses at an introductory level the conditions where each of the techniques may be applied, and gives brief guidelines for selecting between them. The chapter also briefly discusses how to perform a waste load allocation for single and multiple discharge cases and how to calculate the return period. Last is a discussion of toxic concentration criteria. Discussions provided herein are very brief only as necessary to alert the users to important technical issues. More detailed discussion is beyond the scope of this users manual.

Selecting Between Techniques

Each of the three techniques can be applied to perform toxics waste load allocations and no one technique is necessarily preferable to ary other on a theoretical basis. However, all three techniques are not similarly accurate or appropriate in all situations. This section highlights when each technique should be applied.

Continuous Simulation: Continuous Simulation is the most powerful technique but only when sufficient time-series data are available to define the input parameters. The power of Continuous Simulation decreases significantly when data must be synthesized to replace missing historical values. The guidelines for selecting Continuous Simulation as a function of time-series data availability can be summarized as follows:

Time-Series Data Availability	Applicability of Continuous Simulation
All input parameters available and complete	Very high
Only one effluent parameter missing or significantly incomplete	High
Both effluent parameters missing but other data is complete	Fair
All other cases	Poor

Continuous Simulation can be very reliable when analyzing the frequency distribution of concentrations for existing conditions where all parameters are well defined. However, the technique is at best fair when projecting concentrations for future treatment alternatives because the sequential nature of effluent flow and concentration cannot typically be defined as treatment changes. If the user is uneasy about this problem it is possible to use Continuous Simulation to simulate the concentration distribution for existing conditions and the Monte Carlo technique for projecting the impact of future treatment alternatives.

Monte Carlo: Monte Carlo analysis has the least stringent input requirements of any of the three techniques and therefore the widest applications. It is best used in situations with limited cross and serial correlation of parameters; in these cases Continuous Simulation is preferred where data are available. It can be applied in cases where the available data are inadequate for either Continuous Simulation or for Log Normal analyses. However, if the data are insufficient or inadequate the reliability of results must be considered. Any of three standard statistical distributions - uniform, normal, or triangular - should be used whenever possible to describe input data; but data defined distributions can also be used. Since data defined distributions can be used for even the most limited data sets, care should be taken to ensure that sufficient data exists to provide meaningful results.

Log Normal: The Log Normal technique is attractive because it requires far less computational expense than the other two techniques. However, it can only be applied for waste load allocation with single discharges and where all input parameters have been shown to be log normally distributed, The Log Normal technique can also be used as a lower-cost screening technique when parameters are not all log normally distributed before conducting more complex analyses with Continuous Simulation or Monte Carlo. In examining the consistency of data to log normality special emphasis should be placed on the "tail ends" of the distribution curves. It is typically at the extremes of the input distributions where water quality problems occur and thus where the assumption of log normality must be the most rigorously justified.

Allowable Effluent Loads

Water quality criteria are currently defined for maximum concentrations of a constituent for a three year return period. For acute toxicity, the instream concentration should not exceed 0.3 times the toxic concentration level (or 0.3 toxic units acute) more than once in three years. Although the critiera were determined for a one hour duration, the criterion will generally be interpreted on a daily averaged basis because more frequent calculations cannot be practically supported by data. For chronic toxicity, the instream concentration for a four day average should not exceed the chronic toxic level (1.0 toxic units chronic) similarly more than once in three years. Allowable effluent loads should be calculated to maintain these conditions.

The waste load allocation process determines the effluent concentration and flow that will result in a three year return period for the desired in-stream concentration. DYNTOX allows two ways of determining the allowable effluent load, both of which are equally valid and consistent:

1) inspection of the return period corresponding to a desired in-stream concentration;

2) inspection of in-stream concentrations corresponding to a desired return period.

Using the first method, a user performing an acute waste load allocation would inspect the return period for an in-stream concentration of 0.3 tua. If the return period is less than three years, the effluent load is too large and must be decreased. If the return period is greater than three years, the effluent load may be increased. The waste load allocation process using this technique consists of finding the largest effluent load that will result in an in-stream return period for three years or greater for the water quality criterion.

The second method for performing a waste load allocation is to determine the in-stream concentration that has a three year return period. For the acute toxicity example, the user inspects the in-stream concentration with a three year return period. If this concentration is greater than 0.3 tua, the effluent load is too large and must be decreased. If the in-stream concentration with a three year return period is less than 0.3 tua, the effluent load may be increased. The waste load allocation process using this technique consists of finding the largest effluent load that will result in an in-stream three year return period concentration less than or equal to the water quality criterion.

Multiple Discharges

Establishing allowable toxic loads among multiple discharges in one system involves technical and policy issues handled differently by different states. One simple approach is to calculate the maximum allocations successively, upstream to downstream, ignoring the inherent upstream preference. A second approach would be to require consistent removal efficiencies from all discharges ignoring that the assimilative capacity may not be fully used in all river segments or allowing individual increases. A third would be to assume no decay and allocate proportional to flow. The list of options is extensive. The specific policy and procedure is a State issue which involves technical, policy and political consideration. However, DYNTOX can generally be adapted to address most any State policy.

In the illustrative examples included in this Appendix, a very simple approach is used wherein allocations are conducted successively upstream to downstream. This procedure was chosen only to illustrate the use of DYNTOX and in no way represents a recommended procedure for allocating among multiple discharges.

Calculating the Return Period

Two common methods exist to calculate the return period for a given concentration from probabilistic modeling. They are termed herein as:

1) the percentile method

2) the extrema method

The percentile method uses a listing of all in-stream concentrations and ranks them. The return period for a concentration is then calculated based upon percentile occurrence. In the extrema method, only annual extreme values are used in the ranking. The return period calculated from these two methods are equally valid statistical representations, but neither necessarily predicts annual occurrence frequency.

The percentile method assumes that all violations of the in-stream criteria are independent from each other. Every exceedance of the criteria is treated equally, including multiple violations in the same year. Results from this method therefore represent an "average" return period. The disadvantage to this technique is that multiple violations related to the same extended event (e.g. drought river flow) are treated as separate events, which could lead to an estimation of the recurrence interval which is more frequent than actually characteristic. The advantage to the percentile technique is that multiple, independent violations occurring in the same year are correctly incorporated into the return period analysis.

The extrema method uses only the largest concentration for each year in calculating the return period value. This technique predicts the return period for an annual extreme value and has the advantage of not "double counting" multiple violations that are caused by the same event. The disadvantage to the extrema method is that when multiple independent violations occur in the same year, only one violation is considered in the return period analysis. This can lead to an estimate of the return period which may be longer than truly characteristic.

For the DYNTOX examples provided in this report, as for all analyses conducted using DYNTOX, the percentile method is used. Users have the ability to perform extrema analysis by running Continuous Simulation one year at a time and manually tabulating the extreme in-stream concentration for each year. Investigations are now being conducted to establish the appropriate application of the two techniques and the need to adapt DYNTOX to more directly compute the extrema method.

In either case the degree of confidence that can be placed in model results is directly related to the amount of input data available and the return period for the concentration of interest. In general, the longer the return period the more data that is required. If recurrence intervals of 10 to 20 years are desired, input data should accurately define the 30 year return value of all input parameters in order to estimate the probability of such rare events. Although the program will provide results using an inadequate data base, these results should not be used in performing waste load allocations.

Toxic Concentrations

Toxic concentration criteria for waste load allocation can be determined by two methods:

- o chemical specific
- o effluent toxicity testing

The chemical specific method involves using scientific toxicity data for a particular toxicant and establishing the concentration level of acute and chronic toxicity. Limited consideration is typically given to synergistic and antagonistic effects with other parameters. On the other hand, effluent toxicity testing uses an operational approach. Bioassays are performed with the effluent at different dilution levels to determine its toxicity as a whole. Its toxicity is then defined in toxic units where one unit equals the least concentrated dilution which caused the test endpoint. Other levels of concentration are described in toxic units which are multiples of this dilution. Detailed discussion of these concepts is not appropriate for this users manual and the reader is referred elsewhere (EPA, 1985). However some comments are appropriate.

Whole effluent toxicity testing has many advantages because it directly considers site specific effluent toxicity and inherently considers multi-parameter effects. However, on the downside:

- o almost no toxic unit data exists for upstream water quality
- o defining combined effects of multiple effluents is difficult
- o quantifying in-stream decay of toxicity is also difficult.

In contrast, chemical specific toxic criteria are simple to use and apply. They are limited however because they:

- o are not site specific
- o do not consider synergistic effects
- o do not consider antagonistic effects

Both options have advantages and disadvantages. The reader is encouraged to research these issues in more appropriate technical documents (e.g. EPA, 1985).

VII. REFERENCES

DiToro, D. M. Probability Model of Stream Quality Due to Runoff. Journal of Environmental Engineering, ASCE, Vol. 110, No. 3, June, 1984.

Fiering, M.B. and B. Jackson. Streamflow Synthesis, American Geophysical Union, 1971.

Freedman, P.L. and R.P. Canale. Modeling Uncertainty and Variability for Waste Load Allocations. LTI, Limno-Tech, Inc., prepared for USEPA Monitoring and Data Support Division, August, 1983.

SAS Institute Inc. SAS User's Guide: Basics, 1982 Edition. Cary, North Carolina, 1982.

Thomann, R.V. Systems Analysis and Water Quality Management. McGraw-Hill, New York, 1972.

USEPA Office of Water Technical Support Document for Water Quality - based Toxics Control. September, 1985.

USEPA Storet User Handbook. USEPA, Washington, D.C., 1982.