

EPA's COMPOSITE MODEL FOR LEACHATE  
MIGRATION WITH TRANSFORMATION PRODUCTS

**EPACMTP: USER'S GUIDE**

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## PREFACE

This document presents guidance for the use of EPA's Composite Model for leachate migration with Transformation Products (EPACMTP) computer code. EPACMTP is a simulation model for subsurface fate and transport of contaminants released from land disposal sites. EPACMTP is designed to predict the groundwater exposure in a domestic drinking water receptor well associated with such releases. The model is applied to support development of regulations for management and disposal of hazardous wastes. Simulations are performed using probabilistic input specifications based on nationwide data. The model is designed to be used for generic, nationwide assessments using Monte Carlo simulation techniques; it is not intended for site-specific applications. EPACMTP extends and enhances the modeling approach adopted for the 1990 Toxicity Characteristic (TC) Rule promulgated by the U.S. Environmental Protection Agency in March 1990. For this rule, the Agency used EPACML (EPA's Composite Model for Landfills) to estimate the potential human exposure to hazardous chemicals leaching from land disposal facilities. EPACML accounts for first-order decay and linear equilibrium sorption of chemicals, but disregards the formation and transport of transformation products. The analytical groundwater transport solution technique employed in EPACML further imposes certain restrictive assumptions; the solution can handle only uniform, uni-directional groundwater flow and thereby ignores the effects of groundwater mounding caused by leakage from the waste site on contaminant migration. To address the limitations of EPACML, the modeling approach has been enhanced and implemented in EPACMTP. The EPACMTP modeling approach incorporates greater flexibility and versatility in the simulation capability; the model explicitly can take into consideration: (i) chain decay reactions and transport of daughter and grand-daughter products, (ii) the change to groundwater velocity as a result of water-table mounding, (iii) finite source as well as continuous source scenarios, and (iv) metals transport through linking with the MINTEQ metals speciation model.

In addition to enhancing the simulation capabilities of the EPACMTP computer code, the Agency has also re-evaluated and updated the data used in the nationwide Monte Carlo modeling assessment. The Agency has evaluated additional data from surveys of actual waste sites<sup>1</sup> and other pertinent studies. Based on the additional data sources, the Monte Carlo methodology as well as the frequency distributions of individual model input parameters have been revised and enhanced. The Monte Carlo methodology implemented in the current version of EPACMTP uses a regional, site-based approach which directly accounts for any dependencies between the geographical location of a waste site and the corresponding regional climatic and hydrogeological characteristics.

In parallel with enhancing the model computer code and Monte Carlo methodology, the Agency has conducted various verification and field validation studies. Individual components and modules of the computer code have been verified against existing analytical and numerical solutions, as documented in the EPACMTP Background Document. The modeling approach and solution techniques have been reviewed by the Science Advisory Board; their implementation has been reviewed and tested by the EPA's Office of Research and Development and outside reviewers. The Agency has field-tested the model at a number of actual field sites for which adequate source and site characterization data, as well as plume monitoring data, were available. These sites include the Borden landfill research site in Ontario, Canada; a pesticide contaminated site on Long Island, New York; a pesticide monitoring field site near Kansas City,

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<sup>1</sup> U.S. Environmental Protection Agency, Industrial Subtitle D Facility Study (Telephone Survey), October 20, 1986; U.S. Environmental Protection Agency, Solid Waste Disposal in the United States: Report to Congress, Office of Solid Waste and Emergency Response, EPA/530-SW-88-011, October, 1988

Kansas; and an electric utility waste disposal site in New York State. In all these cases, EPACMTP was found to yield reasonably good predictions of actual plume concentrations. The implementation and documentation of the model have been revised also in response to critical evaluations of the modeling approach by various public interest and industry groups. In response to these comments, the Agency has conducted additional testing of the model, as well as reconsidered and revised various aspects of the modeling procedures, e.g., options for placement of the receptor well down-gradient from the waste site were revised to remove a bias towards larger waste sites.

The present version of the model represents a development effort which has spanned more than six years. Although a considerable effort has been expended on developing and testing the model, EPACMTP, like any computer model, provides a simplified representation of conditions and processes that may be encountered at actual waste sites. Although there is much ongoing research in the area of subsurface fate and transport processes, there is no clear consensus on how to represent all of these processes in a computationally efficient way, particularly in the framework of a generic model such as EPACMTP. Furthermore, the lack of detailed site characterization data on, for instance, heterogeneities and fractures on a nationwide basis, inevitably imposes limitations. EPACMTP therefore represents a balance and compromise between the evolving understanding of subsurface fate and transport processes and the ability to reproduce these processes in a computationally efficient model. Therefore, the use of the model for site-specific applications, where heterogeneities and other complexities might make it unsuitable, is discouraged.

## ABSTRACT

The EPA's Composite Model for leachate migration with Transformation Products (EPACMTP) code, is used by EPA (the Office of Solid Waste) to simulate the fate and transport of contaminants leaching from a land-based waste management unit through the underlying unsaturated and saturated zones. EPACMTP replaces EPACML as the best available tool to predict potential exposure at a downstream receptor well. EPACMTP offers improvements to EPACML by considering: 1) the formation and transport of transformation products; 2) the impact of groundwater mounding on groundwater velocity; 3) finite source as well as continuous source scenarios; and 4) metals transport.

Fate and transport processes simulated by the model include: advection, hydrodynamic dispersion, linear or nonlinear sorption, and chain-decay reactions. In cases where degradation of a waste constituent yields daughter products that are of concern, EPACMTP accounts for the formation and transport of up to six different daughter products. The composite model consists of a one-dimensional module that simulates infiltration and dissolved constituent transport through the unsaturated zone, which is coupled with a three-dimensional saturated zone module. The saturated zone module consists of a three-dimensional groundwater flow and a three-dimensional transport sub-module. The saturated zone groundwater flow sub-module accounts for the effects of leakage from the land disposal unit and regional recharge on the magnitude and direction of groundwater flow. The saturated zone transport sub-module accounts for three-dimensional advection and dispersion, chain decay reactions with up to seven different chemical species (i.e., parent with up to six daughter products), and linear or nonlinear equilibrium sorption.

The fate and transport of dissolved waste constituents in the subsurface depends on the chemical properties of the contaminants as well as on hydrogeological and other parameters. The effect of uncertainty or variability in these parameters on receptor well exposure estimates can be taken into account using the Monte Carlo simulation technique. The Monte Carlo simulation module used in EPACMTP is based on the Monte Carlo module in EPACML. The Monte Carlo Methodology has been enhanced by incorporating a site-based approach which accommodates dependencies between parameters and accounts for regional differences in climatic and hydrogeologic conditions, and which can accommodate finite as well as continuous sources.

This document is intended as a user's guide for EPACMTP; for details of the mathematical techniques employed, the reader is referred to EPACMTP background document for the unsaturated and saturated zone and Monte Carlo modules (U.S. EPA, 1996b). Details on the finite source modeling procedure and background and methodology for the fate and transport assessment of metals are presented in separate background documents (U.S. EPA, 1996c and U.S. EPA, 1996d, respectively).

## **DISCLAIMER**

The work presented in this document has been funded by the United States Environmental Protection Agency. Mention of trade names or commercial products does not constitute endorsement or recommendation for use by the Agency.

### **WARNING**

EPACMTP was developed for regulatory purposes for implementation on a nationwide basis using the Monte Carlo simulation procedure, and the code is not suitable for site-specific use. The model does not account for site heterogeneities, complicated source conditions, and several other site-specific conditions which may be encountered at actual waste sites.

## ACKNOWLEDGMENT

A number of individuals have been involved with the development of the EPACMTP model. Dr. Zubair Saleem of the U.S. EPA, Office of Solid Waste, provided overall technical coordination and review throughout this work.

Drs. Peter Huyakorn and Jan Kool of HydroGeoLogic, Inc. developed the unsaturated zone module used in the composite model. Dr. Edward Sudicky, Robert McLaren and Rene Therrien of the University of Waterloo developed the saturated zone module. Neil Blandford of HydroGeoLogic, Inc. developed the Monte Carlo module of EPACMTP, based on a similar module in EPA's Composite Model for Landfills (EPACML). Dr. Carlos Marin of Ambiotec Environmental Consultants provided overall technical support for the site-based Monte Carlo conceptualization of the model and the finite source methodology. Raj Lingam and Omar Abdi of HydroGeoLogic, have implemented and tested the current version of the EPACMTP model. The fate and transport methodology for metals is under development in cooperation with the EPA ORD Environmental Research Laboratory in Athens, GA. Drs. Nam-Sik Park and Yu-Shu Wu modified and implemented the model for metals in cooperation with Jerry Allison of Allison Geoscience and staff at the EPA Environmental Research Laboratory in Athens, GA.

## **EPACMTP Quick Start Guide**

This Quick Start section is intended to get new users up and running with EPACMTP quickly. It is not a replacement for the complete User's Guide. To fully understand the model capabilities and assumptions, and how to use EPACMTP effectively, all users should consult this EPACMTP User's Guide, the Background Document (U.S. EPA, 1996a, b, c).

The EPACMTP modeling software consists of:

EPACMTP: The Monte Carlo fate and transport model

POSTCMTP: A menu-driven post-processor for analyzing EPACMTP model results.

The Quick Start guide tells you how to install the software and how to use the model and the pre- and post-processors.

### ***Computer Requirements***

To install and run EPACMTP, you must have an MS-DOS 80386 or better PC with at least eight (8) megabytes of RAM memory. A fast Pentium computer is highly recommended. About 1.5 megabytes of free disk space is required to install the software. Finite source modeling runs may require up to 20 megabytes of additional disk space for temporary files.

In order for EPACMTP to operate correctly, your CONFIG.SYS file should contain the following commands:

```
FILES = 20 (or more)
DEVICE = ANSI.SYS
```

### ***Installation Procedure***

The installation is controlled through a utility program, INSTALL.EXE on the distribution disk. To install follow these steps:

- Insert the distribution diskette in the appropriate disk drive. This is the *source* drive (usually *a:*)
- Make the source drive the current drive, by typing '*a:*' at the DOS prompt
- Type '*INSTALL a: c:*' where *a:* represents the source drive and *c:* represents the target drive.

The installation program will automatically copy the contents of the *a:* drive into a directory call "EPACMTP" on you *c:* drive.

- That's it!

After installation is complete, some information on EPACMTP will be displayed on-screen. This information can be viewed again later by typing '*MODL-INFO*'.

## **RUNNING EPACMTP**

To setup an EPACMTP run you must first create an ASCII data input file. Detailed instructions for this are provided in Appendix A. To create a new input file for another problem, you can use a text editor to modify an existing data input file.

Sample data files are provided in the EPACMTP directory. Consult the file FILES.LST for a list of the file names. To run EPACMTP, simply type '*EPACMTP*' which will bring up the Main Menu screen. From the Main Menu, using the arrow keys, select 'Run' and hit [*RETURN*]. This will give you the Run Option screen. To run the model, select the (C)ommand line mode option by pressing the letter C. Then enter the name of the input data file and press [*RETURN*].

- You must give complete DOS file names
- EPACMTP will use the same name as the data input file, but an extension of '*.out*', to create the model output file

When EPACMTP is running in Monte Carlo mode, an iteration counter and estimated completion time are displayed on-screen. This will show the progress of the Monte Carlo simulation. Do not be alarmed when a run takes a long time, especially in the case of finite source simulations.

## **USING THE POST-PROCESSOR**

EPACMTP generates a number of output files. The main output file (extension '*.out*') contains a listing of the data input. The Monte Carlo output is stored in files with extension of '*.cdf*' (for continuous source analyses) and '*.sat*'. (for finite source analyses). The POSTCMTP post processor allows you to graphically analyze the modeling results contained in these output files.

### ***POSTCMTP Post-Processor***

POSTCMTP is a menu-driven utility for graphically analyzing EPACMTP Monte Carlo results. It also has the capability of plotting graphs on a wide variety of printers and plotters, or saving a graph on disk in HPGL format for importing into various word processing and/or desktop publishing programs.

To start POSTCMTP, type '*POSTCMTP*' at the DOS prompt or select 'Plot' from the main menu of EPACMTP. The main menu of POSTCMTP presents three primary options:

- (C)ontinuous Source Analysis
- (F)inite Source Analysis
- (I)nititalize Plotting Device

The very first time you run POSTCMTP, you will be taken automatically into the Initialization menu, so we will discuss that first.

### Initialize Plotting Device

The initialization menu allows you to select the type of printer or plotter and the parallel (LPT:) or serial port (COM:) through which the printer or plotter is connected to your PC. If you select a printer, you will also be asked for the desired density of the printed graph. A higher density will result in better quality, but also slower printing. After you make the initial setup, the information is stored by POSTCMTP. To change any of the settings, you must go through the (I)nititalize menu again.

### Continuous Source Analysis

After you select (*C*)ontinuous Source from the main menu, you are prompted for the name of the Monte Carlo output file. Enter the root filename only, without extension! The main options on the Continuous Source menu are:

- (*G*)raph: View the DAF or CDF curve, and optionally send it to a printer or plotter
- (*S*)pecify: Enter a probability level and get the corresponding DAF value, and vice versa
- (*N*)ew File: Enter a new filename to analyze

If you select the (*G*)raph option, the cumulative probability function (CDF) of the normalized receptor well concentration (i.e., the inverse of DAF) will be drawn on-screen.

After the plot is completed, a number of additional options appear at the bottom of the screen. These include (*H*)ard Copy, to send the plot to your printer or plotter, and (*S*)ave which allows you to save the plot on disk for later viewing, or in HPGL format. The latter allows you to import the graph directly into reports and documents by importing the HPGL plot file as a graphic into your wordprocessor. Note that printing to a laser printer at high resolution is quite slow; it may take 5 minutes per plot.

### Finite Source Analysis

After you select (*F*)inite Source from the main menu, you will first be prompted for the name of the Monte Carlo output file. Enter the filename only, without extension!. The main options on the Finite Source menu are:

- (G)raph:* View the graph of leachate versus waste concentrations at the selected protection level
- (S)pecify:* Select the desired protection level, or get the maximum leachate concentration for a given waste concentration
- (N)ew file:* Enter a new file name to analyze.

If you select the *(G)raph option*, a plot of leachate versus waste concentration corresponding to the selected protection level will be drawn on-screen. The default protection level is 85%.

After the plot is completed, a number of additional options appear at the bottom of the screen. These include *(H)ard Copy*, to send the plot to your printer or plotter, and *(S)ave* which allows you to save the plot on disk for later viewing, or in HPGL format. The latter allows you to import the graph directly into reports and documents by importing the HPGL plot file as a graphic into your wordprocessor. Note that printing to a laser printer at high resolution is quite slow; it may take 5 minutes per plot.

The *(S)pecify* option allows you to change the default protection level used in generating the graph of leachate versus waste concentrations.

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## 1.0 INTRODUCTION

The USEPA Office of Solid Wastes (OSW) has developed a probabilistic (Monte Carlo) groundwater flow and transport modeling approach to assess potential exposure of groundwater to toxic chemical constituents in wastes that are managed in Subtitle D industrial waste management units under RCRA regulations. The exposure to groundwater is expressed as concentrations of potential contaminants at drinking water well (receptor well) located downgradient of the waste disposal facility. This modeling methodology has been incorporated into the EPA's Composite Model for Leachate Migration with Transformation Products code (EPACMTP; EPA, 1996 a,b,c,d). The OSW of the U.S. EPA has recently applied EPACMTP, as a general fate and transport model, to establish regulatory levels for concentrations of chemicals in the above wastes under the proposed Hazardous Waste Identification Rule (HWIR; EPA, 1995).

EPACMTP simulates a one-dimensional, vertically downward flows and transport of contaminants in the unsaturated zone underneath a waste disposal unit, and 3-D or 2-D groundwater flow and contaminant transport in the underlying saturated zone. The model accounts for the following processes affecting contaminant fate and transport: advection, hydrodynamic dispersion, linear or nonlinear equilibrium sorption, chained first-order decay reactions, and recharge dilution in the saturated zone. EPACMTP incorporates a Monte Carlo module which allows for the assessment of uncertainty in receptor well concentrations due to variations in the model input parameters.

This document is prepared to facilitate the use of EPACMTP as an analytical tool. Section 1.1 provides general background information to direct the user through this document. Section 1.2, outlines the model capabilities and limitations. Practical code requirements and installation procedures are provided in Section 1.3. To promote further utilization and future enhancements of the model, the user is encouraged to direct questions and comments to EPA's contact person. This information is provided in Section 1.4.

### 1.1 ORGANIZATION OF THE DOCUMENT

This report is prepared to facilitate the use of EPACMTP as an analytical tool. It provides the user a sequentially organized instructions to prepare an input file for EPACMTP. It also presents brief discussion on some of the key concepts of the model, particularly, with regard to estimation of input parameters as well as model output analysis. This document, alone, does not contain the background information that is necessary for a thorough knowledge and understanding of theoretical concepts and methodologies of EPACMTP components. Therefore, it is strongly recommended that the user read this and all other technical documentation of EPACMTP (EPA 1996 b, c, d) to achieve a comprehensive understanding of the model. The rest of this section provides general information to direct the user through this document. Section 1.2, outlines the model capabilities and limitations which the user must be familiar with before using the model for any applications. Practical code requirements and installation procedures are presented in Section 1.3. To promote further utilization and future enhancements of the model, the user is encouraged to direct questions and comments to EPA's contact person. This information is provided in Section 1.4. This report is divided into the following four parts.

## Part 1: Simulation Objectives of the Model

## Part 2: Waste and Waste Management Unit Characterization

## Part 3: Fate and Transport Simulation in the Subsurface

## Part 4: Model Output Processing and Analysis

These parts represent the sequence of general considerations and information gathering steps that are required to develop an input file for the EPACMTP code. The material covered in each part is briefly described in this section. The major components, options and considerations for each part of the process are summarized in Table 1.1. This table also provides a reference column that gives the specific section of this report where the user can get details on specific items.

The first part addresses model input parameter which determine the general settings of the model under which fate and transport simulations are performed. Among these parameters are the model's execution mode (Monte Carlo or deterministic), waste management unit type (e.g. landfill, surface impoundment), source release scenario (continuous or finite source) etc. This group of parameters are identified in the input file by their group code, GP which stands for general parameters. Chapter two focuses on issues related to source release scenarios and Chapter 3 addresses other parameters that determine the general setting of the model.

Part 2 addresses parameters required to characterize waste management unit characteristics (e.g., area, depth, geographical location and climatic zone) as well as waste characteristics (e.g., volume, density and concentrations in the waste and leachate). This group of variables are called source-specific parameters and are identified in the input file by their code SS. Described in Part 2 of the report also are the chemical-specific parameters identified in the input file by the code CS. This group of variables provide constituent specific information such as hydrolysis rates, diffusion coefficient, organic carbon distribution ( $k_{oc}$ ) etc.

Part 3 of the document focuses on model variables that characterize unsaturated zone (US) and saturated zone (AS) parameters. The letters shown in the brackets are the identification codes for these two groups of parameters in the input file respectively. Unsaturated zone parameters include depth to water table, saturated hydraulic conductivity, soil moisture characteristic parameters dispersion etc. Examples of the saturated zone parameters include aquifer thickness, hydraulic conductivity, hydraulic gradient, dispersivity and receptor well location.

Part 4 of the report addresses issues regarding model output processing and analysis. It describes how the output of the model, receptor well concentrations, are used to build probability distribution function which defines different levels of protection.

Appendix A contains detailed instructions on how to prepare an EPACMTP input file. The instructions are designed to guide the user, step by step, through the process of creating an input data file. The task of input file preparation would even be easier in the near future when a Windows-based EPACMTP preprocessor with graphical user interface is available. A DOS-based program is currently available for post processing of model results and is also presented in Appendix A. Sample input and output files for a Monte Carlo simulation scenario for landfills are presented in appendix B. Appendix C provides frequency distributions for key EPACMTP input parameters.

Table 1.1 Summary of the Components of EPACMTP Model

Component	Input File Code*	Options	Consideration (s)	Reference Section
A. Source-Release Scenario	GP	<ul style="list-style-type: none"> <li>● Continuous</li> <li>● Finite</li> </ul>	<ul style="list-style-type: none"> <li>● Waste management scenario of concern</li> </ul>	2.0
B. Methodology of Simulation	GP	<ul style="list-style-type: none"> <li>● Deterministic</li> <li>● Monte Carlo</li> </ul>	<ul style="list-style-type: none"> <li>● Single values for specific parameters</li> <li>● Probability distributions for specific parameters</li> </ul>	3.0
C. Waste and Waste Management Unit Characteristics	SS	<ul style="list-style-type: none"> <li>● Landfill</li> <li>● Surface impoundment</li> <li>● Waste pile</li> <li>● Land application unit</li> </ul>	<ul style="list-style-type: none"> <li>● Active life</li> <li>● Dimensions</li> <li>● Waste value and leachate concentration</li> <li>● Climatic/hydrogeologic Characteristics</li> </ul>	4.0
D. Contaminant Type	CS	<ul style="list-style-type: none"> <li>● Organic</li> <li>● Metal</li> </ul>	<ul style="list-style-type: none"> <li>● Transformation Products</li> <li>● Sorption Characteristics (linear/nonlinear)</li> </ul>	5.0
E. Unsaturated zone module	US	Flow <ul style="list-style-type: none"> <li>● Steady-state (1D)</li> </ul> Transport <ul style="list-style-type: none"> <li>● Steady-state</li> <li>● Transient</li> <li>● Sorption (linear/nonlinear)</li> <li>● Decay</li> </ul>	<ul style="list-style-type: none"> <li>● Depth to water-table</li> <li>● Soil characteristics</li> </ul>	6.0
F. Saturated zone module	AS	Flow <ul style="list-style-type: none"> <li>● Steady-state (2D or 3D)</li> </ul> Transport <ul style="list-style-type: none"> <li>● Steady-state</li> <li>● Transient</li> <li>● Linear sorption</li> <li>● Decay</li> </ul>	<ul style="list-style-type: none"> <li>● Aquifer characteristics</li> <li>● Saturated thickness</li> <li>● Ambient groundwater gradient</li> </ul>	7.0
G. Receptor Well Location	AS	<ul style="list-style-type: none"> <li>● Within plume</li> <li>● Anywhere downgradient</li> <li>● Along plume centerline only</li> </ul>	<ul style="list-style-type: none"> <li>● (x) distance from waste unit</li> <li>● (y) distance from plume centerline</li> <li>● (z) well depth</li> </ul>	7.13

\*See Appendix A

## 1.2 EPACMTP CAPABILITIES AND LIMITATIONS

The EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP) comprises four major components:

- A module that performs one-dimensional analytical and numerical solutions for water flow and contaminant transport in the unsaturated zone underlying a waste management unit.
- A numerical module for steady-state groundwater flow subject to recharge from the unsaturated zone.
- A module comprising analytical and numerical solutions for contaminant transport in the saturated zone.
- A Monte Carlo module for assessing the effect of uncertainty or variations in model parameters on predicted contaminant concentrations in a receptor well.

A cross-sectional view of the subsurface system modeled by EPACMTP is shown in Figure 1.1. The subsurface consists of an unsaturated zone underneath a waste unit, and an underlying water table aquifer. Contaminants move vertically downward through the unsaturated zone to the watertable. EPACMTP allows for the simulation of flow and transport in the unsaturated zone and in the saturated zone, separately or combined.

To use the model correctly, the user must be aware of the model capabilities and, perhaps more importantly, its limitations. The EPACMTP code is capable of simulating the fate and transport of dissolved contaminants from a point of release at the base of a waste disposal unit, through the unsaturated zone and underlying groundwater, to a receptor well at an arbitrary downstream location in the aquifer. The code accounts for the major mechanisms affecting contaminant migration, including: transport by advection and dispersion, retardation due to reversible linear or nonlinear equilibrium adsorption onto the soil and aquifer solid phase, and bio-chemical degradation processes. The latter may involve chain decay reactions if the contaminant(s) of concern form a decay chain. As is true of any model, EPACMTP is based on a number of simplifying assumptions which make the code easier to use and ensure its computational efficiency. These assumptions, however, may cause application of the model to be inappropriate in certain situations. Therefore, the user should verify whether all assumptions in EPACMTP are appropriate before using the model for any application. The assumptions in EPACMTP are summarized below:

### 1) Soil and Aquifer Medium Properties

It is assumed that the soil and aquifer are uniform porous media, and that flow and transport are described by Darcy's law and the advection-dispersion equation, respectively. The model does not account for the presence of preferential pathways such as fractures and macro-pores. Although the aquifer properties are assumed to be uniform, the model does allow for anisotropy in the hydraulic conductivity.

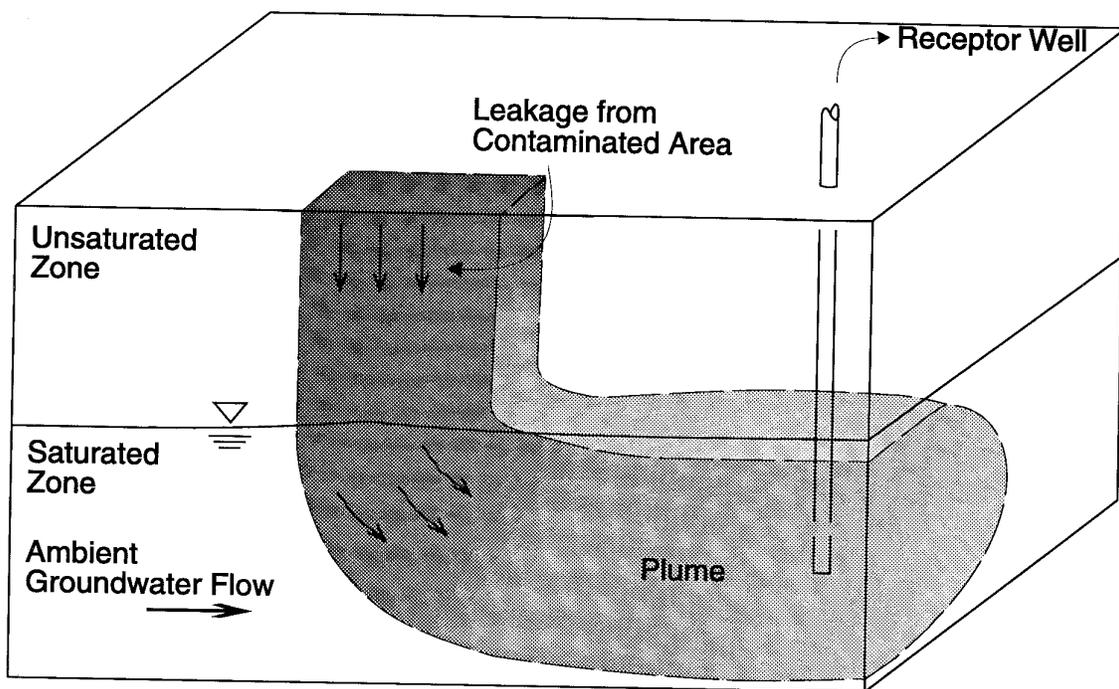


Figure 1.1 A Cross-Sectional View of Subsurface Modeled by EPACMTP.

2) Flow in the Unsaturated Zone

Flow in the unsaturated zone is steady-state one-dimensional vertical flow from underneath the source towards the water table. The lower boundary of the unsaturated zone is the water table. The flow in the unsaturated zone is predominately gravity-driven, and therefore the vertical flow component accounts for most of fluid flux between the source and the water table. The flow rate is determined by the long-term average infiltration rate through the waste management unit. In surface impoundments, it is determined by the average depth of ponding.

3) Flow in the Saturated Zone

The saturated zone module of EPACMTP is designed to simulate flow in an unconfined aquifer with constant saturated thickness. The concept is that of regional flow in the horizontal direction, with vertical disturbance due to recharge and infiltration from the overlying unsaturated zone and waste disposal facility. The lower boundary of the aquifer is assumed to be impermeable. Flow in the saturated zone is assumed to be steady-state.

EPACMTP accounts for different recharge rates underneath and outside the source area. Groundwater mounding beneath the source is represented in the flow system by increased head values at the top of the aquifer. This approach is reasonable as long as the height of the mound is small relative to the thickness of the saturated zone.

4) Transport in the Unsaturated Zone

Contaminant transport in the unsaturated zone is by advection and dispersion. The unsaturated zone is assumed to be initially contaminant-free and that contaminants migrate vertically downwards from the disposal facility. EPACMTP can simulate both steady-state and transient transport in the unsaturated zone, with single species or multiple species chain decay reactions, and linear or nonlinear sorption.

5) Transport in the Saturated Zone

Contaminant transport in the saturated zone is due to advection and dispersion. The aquifer is assumed to be initially contaminant-free and contaminants enter the aquifer only from the unsaturated zone immediately underneath the waste disposal facility, which is modeled as a rectangular horizontal plane source. EPACMTP can simulate both steady-state and transient transport three-dimensional transport in the aquifer. For steady-state transport, the contaminant mass flux entering at the water table must be constant with time. For the transient case, the flux at the water table can be constant or may vary as a function of time. EPACMTP can consider the transport of a single species or multiple species chain decay reactions, and linear sorption.

6) Contaminant Phases

EPACMTP assumes that the dissolved phase is the only mobile phase, and disregards interphase mass transfer processes other than adsorption onto the solid phase. The model does not account for volatilization in the unsaturated zone; this is a conservative approach for volatile chemicals. The model also does not account for the presence of a NAPL (e.g. oil) and transport in gas phase. When a mobile oil phase is present, significant migration may occur within it, so that EPACMTP may underpredict the movement of hydrophobic chemicals.

7) Chemical Reactions

The EPACMTP model represents chemical reactions by adsorption and decay processes.

**Adsorption**

The EPACMTP assumes that sorption of organic compounds in subsurface is represented linear adsorption isotherms in both the unsaturated and saturated zones. It is assumed that the adsorption of contaminants onto the soil or aquifer solid phase occurs instantaneously, and is entirely reversible.

The effect of geochemical interactions is especially important in the fate and transport analyses of metals. For the simulation of metals, EPACMTP utilizes sorption isotherms generated by MINTEQA2 (Allison et al., 1991, a metal speciation model.) MINTEQA2 generates concentration-dependent effective partition coefficients, for various combinations of geochemical conditions. This procedure is described in the background document for the modeling of metals transport (EPA, 1996d).

**Transformation reactions**

EPACMTP accounts for chemical and biological transformation processes. All transformation reactions are represented by first-order decay processes. An overall decay rate is specified for the model, so that the model cannot explicitly consider the separate effects of multiple degradation processes such as oxidation, hydrolysis and biodegradation. The user must determine the overall, effective decay rate when multiple decay processes are to be represented. In order to increase its flexibility, EPACMTP has the capability of determining the overall decay rate from chemical-specific hydrolysis constants using soil and aquifer temperature and pH values.

EPACMTP assumes that the reaction stoichiometry is prescribed for scenarios involving chain decay reactions. The speciation factors are specified as constants by the users (see the EPACMTP Background Document, EPA, 1996b). In reality, these coefficients may change as functions of aquifer conditions (for example, temperature and pH) and/or concentration levels of other chemical components.

## 1.3 CODE REQUIREMENTS AND INSTALLATION PROCEDURE

### Code Requirements

In order to apply the EPACMTP code effectively the user will need:

- A thorough understanding of hydrogeological principles,
- A thorough understanding of solute transport mechanisms,
- An understanding of the principles of Monte Carlo analysis,
- An awareness of the code's capabilities and limitations,
- Familiarity with FORTRAN input format conventions, and
- Familiarity with the editor, operating system, and file handling concepts of the computer system used.

The run-time version of EPACMTP requires an 80386/486 or Pentium based computer with an MS-DOS operating system. A 80387 math coprocessor is required for 386 systems. The computer should be equipped with at least eight (8) megabytes of random access memory (RAM) and a hard disk. To accommodate temporary files created during a model run, the hard disk should have at least one megabyte of free space for Monte Carlo simulations with the continuous source option. For model runs with the finite source option, up to twenty megabytes of free disk space may be required by the model for temporary files.

Users are strongly encouraged to read the entire User's Guide before applying the model. This manual explains the assumptions and approximations used in the model, knowledge of which is a necessary prerequisite for using the model effectively. Instructions for setting up, executing, and analyzing a problem are provided in appendix A.

### Installation Procedure

The EPACMTP program should be executed from a hard disk. To facilitate installation of the files from the distribution diskette onto a computer hard disk, an installation utility (INSTALL.EXE) is provided which automatically copies the necessary files.

To install the software on your hard disk, insert the distribution diskette into your floppy drive (usually "a") and type:

```
a:\install a: c:
```

where *a:* is the drive containing the distribution disk and *c:* is the hard drive.

The installation program will create a directory (default is *c:\EPACMTP*) in which all program files will be installed. In order to run EPACMTP, your CONFIG.SYS file should contain the following lines:

FILES=20 (or greater)  
DEVICE=ANSI.SYS

Consult your MS-DOS manual for more information on configuring the CONFIG.SYS file. Additional information on system configuration will be displayed during the installation procedure and is provided in the README.1ST file on the distribution diskette.

#### **1.4 EPA CONTACT**

For additional information or to submit comments and recommendations, please contact:

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Phone: (703) 308-0467  
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E-mail: [saleem.zubair@epamail.epa.gov](mailto:saleem.zubair@epamail.epa.gov)

**PART 1**

**SIMULATION OBJECTIVES**

## **2.0 SOURCE - RELEASE SCENARIOS**

There are two types of source release scenarios in EPACMTP. They are continuous and finite sources. In a continuous source release scenario, the contaminant leaches out at constant prescribed leachate concentration for an indefinite period of time. In this case, the receptor well concentration eventually reaches a steady-state value. For the finite-source scenario, the release of contaminants occurs over a finite period of time, after which the leachate concentration becomes zero (i.e. all the waste inside the waste management unit has leached out). In addition to the concentration, the receptor well concentration for finite source scenario is also affected by the duration of the source.

The source-release parameter is one of several general parameters (GP) that are designated in the input file. The discussion in this section is restricted to the source-release parameter since it is the most significant general parameter in determining the methodology and approach of the simulation. The designation of other general parameters are addressed in detail in Appendix A.

### **2.1 CONTINUOUS SOURCE SCENARIO**

In the continuous source scenario, the fate and transport model is run in steady-state mode to compute a Dilution-Attenuation Factor (DAF). The DAF is defined as the ratio of source concentration to receptor well concentration. It represents the combined effects of the site, and hydrogeologic and chemical specific parameters on the receptor concentrations. The model run can be conveniently performed using a source leachate concentration value of one, so that the DAF becomes the inverse of the receptor well concentration value. In order to assess the impact of varying site conditions across the nation, the fate and transport model can be coupled to a Monte Carlo module to account for the variability of input parameters. In this way, the model is used to calculate a series of DAF values corresponding to a large number of different model input parameter combinations, reflecting the range of parameter values for different possible waste sites. A probability distribution of DAF values is the result of a Monte Carlo analysis. The resulting DAF values provide a means to identify hazardous versus non-hazardous wastes, based on the DAF values for individual toxic constituents as well as their Health Based Numbers (HBNs) in the waste. See Appendix B for a sample continuous source problem.

### **2.2 FINITE SOURCE SCENARIO**

In the case of a finite source, simulations are performed for transient conditions and the source is assumed to be a pulse of finite duration. The length of the pulse duration, in the case of landfills, is determined by the code based upon the initial amount of contaminant in the landfill, infiltration rate, landfill dimensions, waste and leachate concentration and waste density (EPA, 1996c). For other waste management scenarios (i.e. waste piles, surface impoundments, and land application units), the duration of the leaching period is determined by the waste unit's life time (the default is 20 years for waste piles and surface impoundments, and 40 years for land application units). For the finite source case, the model can calculate either the peak receptor well concentration, or it can calculate an average concentration over a specified period of time. The finite source methodology in EPACMTP is discussed in detail in the finite source background document (EPA, 1996c).

### 3.0 METHODOLOGY OF SIMULATION

Two modes of simulation, deterministic mode and Monte-Carlo mode, are available to the user for applications with EPACMTP. The selection of one of these modes is dependent on: 1) simulation objectives; and 2) the type of data available to simulate the waste management scenario(s) of concern. The deterministic mode uses single values for various source, chemical, and subsurface parameters. This mode is most appropriate for non-probabilistic applications, and simple sensitivity analyses. When using a Monte-Carlo procedure, the source, chemical and subsurface parameters are represented by probability distributions reflecting variations based on national or regional level. Specific capabilities and requirements of EPACMTP for both of these two simulation procedures are presented in the following sections.

#### 3.1 DETERMINISTIC MODE

In order to help the user to appreciate the differences between the deterministic mode and the Monte Carlo procedure, this section describes the capabilities of the EPACMTP in deterministic mode as well as the specific requirements for running the model in deterministic mode.

##### 3.1.1 EPACMTP characteristics in deterministic mode

- Flow is steady-state in both the saturated and unsaturated zones.
- Transport in the unsaturated and saturated zones can be either transient or steady-state.
- If a finite source is being simulated, both the unsaturated and saturated zone transport modules are implemented in the transient mode.
- Each input parameter is assigned a constant value or treated as a derived parameter. An example is the calculation of the partition coefficient ( $k_d$ ) from the fraction organic carbon ( $f_{oc}$ ) and organic carbon distribution coefficient ( $k_{oc}$ ).

##### 3.1.2 Requirements for running EPACMTP in deterministic mode

- The logical variable, MC, in input group GP01 must be set to F(alse).
- If a transient transport in the unsaturated zone is to be simulated, the times at which the concentration profiles in the unsaturated zone are to be written to the output file must be specified by the user.
- If transport in the saturated zone is to be simulated, the user must specify the number of observation wells, and their locations relative to the disposal facility. If a transient run is selected, the user must also specify the time values at which the computed receptor well concentrations are to be written to the output file. Details for setting up a deterministic input data file are presented in Appendix A.

## 3.2 MONTE CARLO MODE

When EPACMTP is used in the Monte Carlo mode, the primary output from the simulation model is a sequence of receptor well concentration values, where each concentration corresponds to the results of one model simulation. For each simulation, a different set of input parameters are generated from appropriate distributions to calculate a receptor well concentration. The Monte Carlo output is then analyzed to derive regulatory DAF values (waste piles, surface impoundments, and application units) or regulatory limits on leachate and waste concentrations landfills. For the continuous source scenario, the DAF is obtained by dividing the source leachate concentration by the receptor well concentration. Each Monte Carlo iteration yields one DAF value for the constituent of concern (one DAF value for each of the transformation products, if the constituent degrades to a daughter product.) Ordering the DAF values from low to high directly yields the DAF cumulative probability distribution (CDF). If appropriate, CDF curves representing different regional distributions may be combined into a single, weighted curve that represents all regions. (See Part 3, Section 2.2 in the Background document for further discussion.)

For the finite source scenario, the post-processing step involves determination of the paired values of leachate concentration,  $C_L$  in the case of landfills, and total leachable waste concentration,  $C_w$ , which satisfy a specified protection level. The procedure is described in the finite source background document (EPA, 1996c). To facilitate the post-processing analysis of Monte Carlo simulations, a separate post-processing program (POSTCMTP) is distributed with the EPACMTP code (see Section 8.0).

### 3.2.1 EPACMTP characteristics in Monte Carlo mode

- Flow in the saturated zone is steady-state in the unsaturated and saturated zones.
- Transport in the unsaturated and saturated zones can be either transient or steady-state.
- If a finite source is being simulated, both the unsaturated and saturated zone transport modules are implemented in the transient mode.
- Prespecified input parameters are represented by probability distributions specified in the input file. It is allowed, however, to specify that a certain parameter is to be treated as a derived variable. An example is the calculation of the waste fraction (ratio of waste volume to facility volume).

### 3.2.2 Requirements for running EPACMTP in Monte Carlo mode

- The logical variable, MC, in input group GP01 must be set to T(true).
- Probability distributions for the stochastic or random parameters must be specified in the EPACMTP data input file.
- If transport in the saturated zone is to be simulated, the user must specify the number of observation wells, and their locations relative to the disposal facility.

If the logical variables CHECK and LDRIV (see Appendix A) are set to TRUE in the Monte Carlo input file, the generated random and derived variables, respectively, are constrained to lie within the upper and lower bounds defined by the user. The randomly generated variables are checked at the end of

subroutine RANGEN, and the derived random variables are checked at the end of subroutine ASSIGN. If any of the constrained values lie outside the specified bounds, the entire Monte Carlo run (except for the reading of the input files) prior to the point of checking is repeated. Random and derived variables that are generated out of bounds are written to the Monte Carlo output file {*OUTPUT*}.BND .

Variables that are to be treated as random must be assigned one of thirteen probability distribution types. The distribution types and their corresponding distribution codes are listed in Table 3.1. The default distribution type for each Monte Carlo variable is discussed in the next chapter. For further information on the various distribution types, consult the EPACMTP Background Document (EPA, 1996b).

### **3.2.3 Regional Site-Based Monte Carlo Approach**

The implementation of the regional site-based Monte Carlo approach in EPACMTP allowed the use of individual waste unit characteristics as well as regional specific climatic and hydrogeologic conditions in the fate and transport simulations. Prior to this approach, model input parameters, such as waste unit area and depth, infiltration and recharge rates, depth to water table, aquifer thickness, etc., were generated from national distributions in which correlation between the geographical location of the waste site and its climatic (infiltration and recharge rate) and hydrogeologic (unsaturated and saturated zone parameters) properties were not preserved. The regional site-based approach is discussed in detail in the EPACMTP Background Document (EPA, 1996b); however, an overview of the methodology is presented here.

The steps involved in the site-based Monte Carlo approach are presented below. Fundamentally, the approach consists of determining the probability distribution of DAF based on the existing Subtitle D waste sites, on the assumption that these sites are an adequate representation of the universe of possible waste sites in the U.S.

Since the the Subtitle D data set only includes the area, volume, location and relative weight of the facility, other data sources are utilized to determine the additional input parameters required to estimate the receptor well concentration for each OPPI site.

The groundwater parameters are obtained by dividing the U.S. into the thirteen hydrogeologic environments developed in the HGDB groundwater study (API, 1989). Each groundwater region includes multiple site- specific combinations of hydrogeologic parameters. In order to assign the groundwater parameters for a given waste site, the hydrogeologic environment is first determined from the geographic location of the waste site. One of the available combinations of groundwater parameters for the hydrogeologic environment is then assigned to the waste site. In the case where the selected groundwater parameter combination has missing values, a joint probability distribution is derived for each groundwater region to generate the missing value as a function of the known values. Given the location of the waste site, the climatic parameters for the nearest climatic center are assigned. The remaining parameters needed to determine the receptor well concentration for a given waste site are generated by using national distributions.

Given a specific realization of input parameters representing a waste site, and the climatic, hydrogeologic, and receptor well characteristics of that site, the corresponding receptor well concentration can be determined. This process is repeated in an iterative manner to construct a probability distribution of receptor well concentrations. During each iteration, a site is selected at random from the Subtitle D data set. The sites are sampled with replacement, i.e., the same site may be selected more than once. The

probability of selecting a specific site depends on the relative weight assigned to that site in the data set.  
. The procedure of the Monte Carlo simulation run is summarized below.

- STEP 1:       Select a Waste Site from Subtitle D Database
- STEP 2:       Generate Recharge and Infiltration for Selected Waste Site
- STEP 3:       Generate Hydrogeologic Variables for Selected Waste Site
- STEP 4:       Generate Remaining Model Input Parameters for Selected Waste Site
- STEP 5:       Calculate the receptor well concentration value for Selected Waste Site
- STEP 6       Repeat Steps 1 through 5 for the number of iterations required, and estimate the national distribution of receptor well concentrations

After Step 5 the receptor well concentration value for a specific realization is obtained. The process is repeated to yield concentration values which represent the nationwide distribution of drinking water exposure concentrations.

Table 3.1 Probability distributions and their associated codes available for use in Monte Carlo module of EPACMTP composite model.

Distribution Type	Distribution Code
1. Constant	0
2. Normal	1
3. Lognormal	2
4. Exponential	3
5. Uniform	4
6. Log10 Uniform	5
7. Empirical	6
8. Johnson SB	7
9. Gelhar Empirical <sup>a</sup>	8
10. Area Transformation <sup>b</sup>	9
11. Vertical Well Position <sup>c</sup>	12
12. Site-based <sup>d</sup>	99
13. Derived Variable	-1

Note: All statistical parameters (mean, standard deviation, lower and upper bounds) are input in standard arithmetic (lineal) space. Appropriate transformations are subsequently performed by the code.

<sup>a</sup>Gelhar's distribution applies only to saturated zone dispersivities (Gelhar et al., 1992).

<sup>b</sup>This distribution applies to municipal Subtitle D landfill areas only.

<sup>c</sup>This distribution applies to the vertical position of the receptor well below the water table only; it is used to specify that the receptor well is located at a fixed depth below the water table.

<sup>d</sup>This distribution applies to parameters that are read directly from an ancillary data file that contains waste locations, volume and area, and corresponding regional climatic and hydrogeological parameters for the site-based Monte Carlo analysis.

**PART 2**

**WASTE AND WASTE UNIT CHARACTERIZATION**

## 4.0 SOURCE-SPECIFIC PARAMETERS

A list of the source-specific input parameters is provided in Table 4.1. EPACMTP can perform Monte Carlo or deterministic analyses for four different types of waste management scenarios: landfills, surface impoundments, waste piles, and land application units. Figure 4.1 shows a schematic, cross-sectional view of the different types of waste units. In terms of the model analysis, each type of waste management scenario is described by a relatively small number of parameters. The differences between waste units are represented by different values or frequency distributions of the source-specific parameters. Source-specific stochastic parameters that may be used by EPACMTP include capacity and dimensions of the waste unit, the leachate concentration, infiltration and recharge rates, pulse duration, fraction of hazardous waste in the waste unit, density of the waste, and concentration of the chemical constituent in the hazardous waste. Data on the area, volume and location of waste units was obtained from the 1986 EPA Survey of Industrial Subtitle D waste facilities in the U.S. This survey is referred to as the OPPI Survey. The derivation of these parameters for each type of waste management unit is described in the EPACMTP background document (U.S. EPA, 1996b).

### 4.1 WASTE UNIT AREA AND DEPTH

The cumulative frequency distributions of the areas of landfill, surface impoundment, waste pile and land application waste units are listed in Table 4.2. These frequency distributions are shown graphically in Figures C1 through C15 in Appendix C.

### 4.2 INITIAL LEACHATE CONCENTRATION (CZERO)

The (initial) leachate concentration for each species in the contaminant decay chain being modeled must be provided by the user. For continuous source (steady-state) simulations, the source concentration of the parent compound is conveniently set to 1.0 (mg/L). Initial daughter product concentrations should be set to zero. For finite source simulations, the (initial) parent leaching concentration should be set to a fixed value. An artificially large value (e.g.  $C_L = 10^6$  mg/L) is recommended for computational convenience. Initial daughter product leaching concentrations should again be set to zero. The actual parent leaching concentration that results in the desired level of protection is determined as part of the post-processing analysis conducted after the Monte Carlo simulation is completed. This procedure is used for organic contaminants and metals with linear sorption behavior. The post processing step takes advantage of the fact that the receptor well concentration for these chemicals varies linearly with the source leachate concentration. For details see the finite source background document (EPA, 1996c).

In the case of metals with nonlinear sorption isotherms, relationship between receptor well concentration and the initial source leachate concentration is nonlinear. Therefore, the model has to be run with different initial source leachate concentrations until the desired protection level is achieved. Because of the nonlinearity the simulation time required is significantly longer than the linear case.

Table 4.1 Source-Specific Variables and Default Distribution Types.

Variable	Units	Distribution Code**	Default Distribution
Waste Site Area ( $A_w$ )	m <sup>2</sup>	99	Regional Site-based
Waste Site Length ( $X_w$ )	m	-1	Derived from area
Waste Site Width ( $Y_w$ )	m	-1	Derived from area
Leachate Concentration ( $C_L$ )	mg/l	0	Constant ( $1 \times 10^{+6}$ for finite source; 1 for continuous source)
Areal Recharge Rate ( $I_R$ )	m/yr	99	Regional Site-based
Infiltration (I)	m/yr	99	Regional Site-based
Ponding Depth*	m	99	Regional Site-based
Thickness of Liner*	m	0	Constant (2 feet)
Hydraulic Conductivity of the Liner*	m/yr	0	Constant ( $1 \times 10^{-7}$ cm/s)
Source Leaching Duration (tp)	yr	-1	Derived
Depth of the Waste Unit (d)	m	99	Regional Site-based
Fraction of Hazardous Waste in the Waste Disposal Unit ( $F_h$ )		4	Uniform
Density of Hazardous Waste ( $P_{hw}$ )	(g/cm <sup>3</sup> )	6	Empirical

\* Required only for surface impoundment if source ponding option is used, i.e. infiltration is set to be a derived parameter.

\*\* See Table 3.1

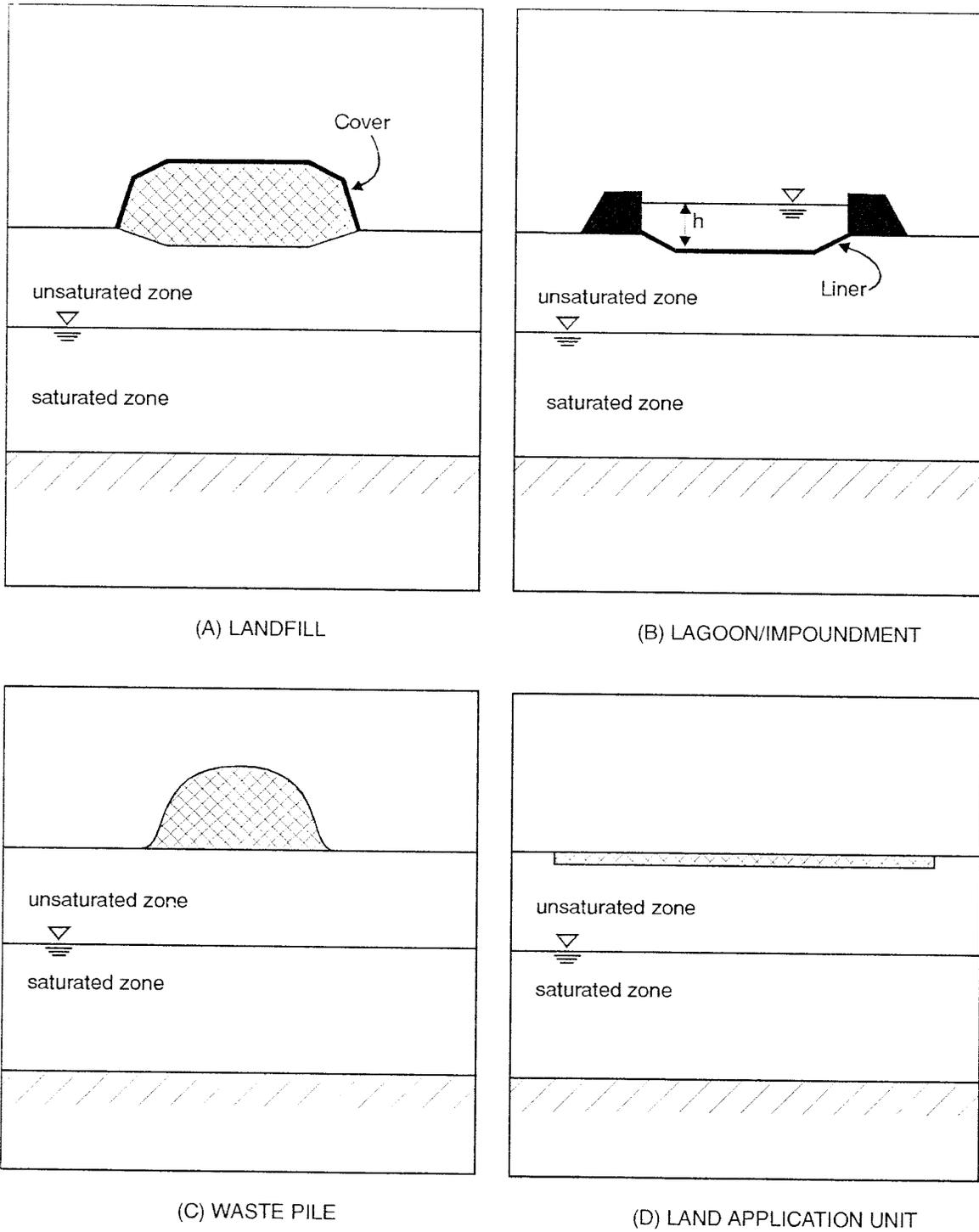


Figure 4.1 Waste Management Scenarios Simulated by EPACMTP.

Table 4.2 Cumulative Frequency Distribution of Waste Unit Area for Industrial Subtitle D Waste Management Facilities.

Landfill		Surface Impoundment		Waste Pile		Land Application Unit	
%	Area (m <sup>2</sup> )	%	Area (m <sup>2</sup> )	%	Area (m <sup>2</sup> )	%	Area (m <sup>2</sup> )
1	44.5	1	24.3	1.8	20.2	1.9	80.9
2	72.8	2	40.5	15.0	28.3	5.1	930.8
5	141.6	5	40.5	25.0	52.6	10.5	3,642
10	809.4	10	80.9	31.4	93.1	20.5	10,117
15	1214	15	161.9	35.5	157.8	31.3	21,813
25	3,683	25	404.7	40.1	230.7	41.0	40,875
35	8,094	35	849.9	45.0	364.2	50.4	97,128
50	16,188	50	2,024	50.1	465.4	59.5	161,880
65	32,3766	65	5,059	60.7	1,133	70.3	273,173
75	60,705	75	8,094	70.5	2,064	80.0	465,405
85	93,081	85	20,235	80.2	5,200	85.1	472,164
90	141,645	90	40,065	85.1	8,992	90.3	105,222
95	221,371	95	81,345	90.0	18,576	95.1	1,942,560
98	554,439	98	234,726	95.0	50,264	99.1	6,879,900
99	1,049,792	99	518,016	99.0	1,011,750		
Min	40.5	Min	13.4	Min	12.1	Min	5.1
Max	3,116,190	Max	60,705,000	Max	2,015,406	Max	8.1107

Note:

The % column denotes the cumulative frequency, i.e.  $P(A \leq \text{Area (m}^2\text{)})$ .

### **4.3 RECHARGE RATES**

The model requires input of the net rate of vertical downward percolation through the unsaturated zone to the water table. The model allows the flow rate through the waste source to be different from the regional average rate. The former is referred to as (source) infiltration rate, the latter is referred to as the recharge rate. The source infiltration rate can be different from the recharge rate for a variety of reasons, including engineering design of the waste site, topography, land use, and vegetation. The recharge rate depends on the regional climatic conditions based on: 1) the proximity of the waste site to one of 97 climatic centers; and 2) the prevalent regional soil type.

Details of the development of the current recharge rate database are presented below. Variations in soil types for determining regional recharge rates have been implemented in the following manner: The Soil Conservation Service (SCS) has a county-by-county soil mapping database. Using this database, the soil classifications in the U.S. were grouped according to the U.S. Department of Agriculture's definitions of coarse, medium, and fine textures. These three categories are represented in EPACMTP by soils equivalent in properties to sandy loam, silt loam, and silty clay loam for the landfill cover materials. An analysis of the SCS database indicates that coarse grained soils, medium grained soils, and fine grained soils represent 15.4 percent, 56.6 percent, and 28.0 percent, respectively, of the soils that have been mapped thus far. The recharge rate was determined separately for each soil type and each of the 97 climatic centers using the HELP model. The recharge rate values for each climatic center are listed in the form of EPACMTP input files at the end of the report. Frequency distributions of recharge rates for different waste management units are provided in Appendix B. The probability of each of the three soil types is assumed to be uniform nationwide. In other words, the soil type and corresponding recharge rate at each modeled waste site is selected in the Monte Carlo analysis from the three different available types, with a weighting equal to their nationwide relative frequency.

### **4.4 INFILTRATION RATES**

Infiltration rates for landfills, waste piles, and land application units were calculated for each of the 97 climatic centers with the HELP model using the procedure and assumptions regarding design characteristics of different types of waste units as described in the EPACMTP background document (EPA, 1996b). In the case of landfills, if the cover type and soil type underneath the unit are the same, the infiltration rate will be the same as the regional recharge rate for that soil type. The infiltration rate values for the landfills, waste piles, and land application units in the modeling database are listed in the form of EPACMTP data input files at the end of this report. The frequency distributions are shown graphically in Appendix C.

For the surface impoundment scenario, the leachate flux rate is computed as a derived parameter, as part of the unsaturated zone flow module. The algorithm is described in the EPACMTP Background Document (EPA, 1996b). In essence, the leachate flux rate is calculated by applying Darcy's law as a function of: (i) impoundment depth, (ii) thickness of a sediment layer at the base of the impoundment, and (iii) hydraulic conductivity of this sediment layer and the underlying soil material.

For the HWIR analyses (EPA, 1995), impoundment depths were obtained from the Subtitle D survey data. All impoundments were assumed to have a sediment layer of 2 feet thickness with a hydraulic conductivity of  $10^{-7}$  cm/s. Although the latter two parameters were taken to be constant, each impoundment in the survey has its own operating depth, and consequently the variation in surface impoundment leachate flux rates is proportional to the variation in operating depths of the impoundments

in the survey. The frequency distribution of the surface impoundment infiltration rate is shown graphically in Appendix C of this document.

#### 4.5 SOURCE LEACHING DURATION

If a finite source simulation is being performed, the duration of the leachate release period must be specified. The duration of the leachate release period is determined in different ways for each of the waste management units. Except for landfills, the release period is determined by the operational life (or active life) of the unit with default values as follows:

Surface Impoundments	-	20 years
Waste Pile	-	20 years
Land Application Unit	-	40 years

In the case of landfills, the waste is left in place after closure of the site, and may continue to leach over a long period of time. The landfill scenario is therefore best handled as follows:

In the Monte Carlo analysis, the pulse duration,  $t_p$ , is treated as a derived parameter and can be set in one of two ways. Specifically, the amount of contaminant leached over the time period  $t_p$  must be equal to the amount of contaminant initially present in the landfill. Method 1, Eqn. 4.1 below, assumes that source contamination,  $C_L$ , is constant until an amount of mass equal to the initial mass is depleted.

$$t_p = \frac{d \cdot F_h \cdot P_{hw}}{I} \cdot \frac{C_w}{C_L} \quad (4.1)$$

where

- $d$  = Depth of waste unit (m)
- $F_h$  = Volume fraction of waste unit that contains waste of concern
- $P_{hw}$  = Density of the waste (g/cm<sup>3</sup>)
- $I$  = Areal infiltration rate (m/y)
- $C_L$  = Leaching concentration of constituent (mg/L)
- $C_w$  = Total leachable waste concentration of the constituent (mg/kg)

Alternatively, Method 2, Eqn. 4.2 below, calculates  $t_p$  from a more rigorous analysis that considers the decrease in the source concentration,  $C_L$ , due to leaching from the waste. In this case, the leachate concentration decreases exponentially, with (EPA, 1996b):

$$C_L = C_L^0 e^{-\left(\frac{I}{d F_h P_{hw}} \frac{C_w}{C_L^0}\right) t} \quad (4.2)$$

where

- $C_L^0$  = Initial leachate concentration (mg/L)
- $t$  = Time (yrs)

Information on the distributions of waste density ( $P_{hw}$ ) and fraction of the waste in the unit ( $F_h$ ) for landfill disposal units is provided in the following sections. During the Monte Carlo analysis, the model simulations are performed for a range of different ratios of  $C_w/C_L$  (or  $C_w/C_L^0$ ). The specific values of  $C_w$  and  $C_L$  (or  $C_L^0$ ) which correspond to a desired level of protection, such as the 90th percentile, are determined following the Monte Carlo run as a post-processing step.

#### **4.6 WASTE DENSITY**

Information on the density of hazardous waste was developed using the densities of 4 major categories of waste (solvents, paints, petroleum products, pesticides) and their contributions to the composition of hazardous wastes in Subtitle D landfills (Schanz and Salhotra, 1992). The results are expressed as an empirical distribution of waste densities, given in Table 4.3. The distribution shows a relatively narrow range of variation, from 0.7 to 2.1 g/cm<sup>3</sup>.

#### **4.7 HAZARDOUS FRACTION OF WASTE**

Data to determine whether a Subtitle D waste exhibits hazardous characteristics are limited. By definition, Subtitle D waste is primarily non-hazardous. The fraction of waste contributed to Subtitle D waste facilities that may exhibit hazardous characteristics is assumed to be randomly distributed and simulated using uniform distribution with lower and upper bounds of 0.036 to 1.0, respectively. The lower bound ensures that the modeled waste unit will always contain a minimum amount of hazardous waste. The lower bound was obtained from an analysis of waste composition in municipal landfills (Schanz and Salhotra, 1992). Note that the input values for waste density and fraction of the waste unit that is occupied by the waste, are required only for the landfill scenario.

#### **4.8 SOURCE TRANSFORMATION RATES**

The model has the capability to account for first-order type chain decay reactions inside the waste source. This requires values for the transformation rate constants of the parent compound and any daughter products. By default, however, the source transformation rate is set to zero, i.e., it is assumed that the contaminant does not degrade inside the waste unit.

Table 4.3 Cumulative probability distribution of waste density.

Waste Density (g/cm <sup>3</sup> )	Cumulative Probability
0.7	0
0.9	0.530
1.12	0.550
1.13	0.551
1.28	0.553
1.30	0.640
1.33	0.728
1.34	0.815
1.36	0.826
1.46	0.904
1.50	0.905
1.62	0.906
1.63	0.994
1.64	0.995
1.65	0.996
2.10	0.998

## 5.0 CHEMICAL-SPECIFIC PARAMETERS

Chemical-specific parameters describe the degradation, adsorptive and diffusive characteristics of each of the chemical species being simulated. The EPACMTP accounts for processes such as decay, adsorption, and diffusion. The model handles the chemical-specific parameters of constituents differently depending on whether the chemical being modeled is an organic compound or a metal. Chemical-specific parameters for the two categories are described below. Chemical-specific parameters of the two chemical categories are described below.

### 5.1 ORGANIC CONSTITUENTS

For organic constituents, EPACMTP accounts for chemical and biological transformations by considering a first order over all degradation rate which may be available directly or derived from acid, base and neutral chemical-specific hydrolysis rates (i.e. Arrhenius equation). The model also takes into account adsorption behavior of organic constituents by calculating a retardation factor based on the organic carbon distribution coefficient ( $k_{oc}$ ) of each constituent and fractional organic carbon in the soil. Other inputs required by the model are reference temperature and constituent drinking water standard. In addition, if a finite source analysis is performed, values are required for the applicable drinking water standard for each constituent, and the exposure averaging period used in the health-risk calculations (e.g. 70 years for a carcinogenic constituent). By default, averaging is not used and the model computes the peak exposure concentration at a downgradient receptor well. In the event that the byproducts are hazardous and their chemical-specific parameters are known, they can be included in the simulation by specifying them to be part of a decay chain. Note that when a multi-species simulation is desired, the necessary chemical-specific parameters must be repeated for all species in the decay chain, NSPECI times. A list of the chemical-specific parameters is provided in Table 5.1.

#### 5.1.1 Hydrolysis Rates

The transport of organic constituents is influenced in part by hydrolysis. Hydrolysis rate constant for each chemical is obtained from:

EPA's Environmental Research Laboratory, Athens, GA. (e.g. EPA, 1993 and Kollig et al., 1990)

Acid- and base-catalyzed hydrolysis rate constants are influenced by pH. The pH dependency is included directly in EPACMTP and the rates are adjusted via the independently derived distribution for pH.

The acid-catalyzed, neutral and base-catalyzed hydrolysis rates are all influenced by groundwater temperature. This effect is quantified using the Arrhenius equation:

$$K_J^T = K_J^{T_r} \exp [E_a/R_g (\frac{1}{T_r + 273} - \frac{1}{T + 273})] \quad (5.1)$$

Table 5.1 Chemical-Specific Variables and Default Distribution Types.

EPACMTP* Parameter	Variable	Units	Distribution Code**	Default Distribution
RLAM 2	Sorbed phase hydrolysis decay rate ( $\lambda_1$ )	1/yr	-1	Derived
RLAM 1	Dissolved phase hydrolysis decay rate ( $\lambda_2$ )	1/yr	-1	Derived
AHYDR 1	Acid catalyzed hydrolysis rate constant	1/mol/yr	0	Constant
NHYDR	Neutral hydrolysis rate constant	1/yr	0	Constant
BHYDR	Base catalyzed hydrolysis rate constant	1/mol/yr	0	Constant
RTEMP	Reference temperature	°C	0	Constant (25°C)
KOC	Normalized distribution coefficient for organic carbon	ml/g	0	Constant
DSTAR	Effective molecular diffusion coefficient	m <sup>2</sup> /yr	0	Constant (0.0 m <sup>2</sup> /yr)
DWS	Drinking water standard (i.e., HBL or MCL)	mg/l	0	Constant
CARC	Exposure averaging period	yr	0	Constant

\* See Appendix A, Table A.2

\*\* See Table 3.1

where

$J$	=	$a$ for acid, $b$ for base, and $n$ for neutral
$T$	=	temperature of the groundwater [ $^{\circ}\text{C}$ ]
$T_r$	=	reference temperature [ $^{\circ}\text{C}$ ]
$K_{a,b}^{T_r}$ and $K_{a,b}^T$	=	the second-order acid- and base-catalysis hydrolysis rate at temperature $T_r$ and $T$ respectively [l/mole-yr]
$K_n^{T_r}$ and $K_n^T$	=	the neutral hydrolysis rate at temperatures $T_r$ and $T$ respectively [1/yr].
$R_g$	=	universal gas constant [1.987E-3 Kcal/deg-mole]
$E_a$	=	Arrhenius activation energy [Kcal/mole]

Note that, using the generic activation energy of 20 Kcal/mole recommended by Wolfe (1985), the factor  $E_a/R_g$  has a numerical value of 10,000.

The acid-catalyzed, base-catalyzed, and neutral hydrolysis rate constants can be combined (Mills et al., 1981) to yield a composite first order hydrolysis rate in the dissolved phase:

$$\lambda_1 = K_a^T [H^+] + K_n^T + K_b^T [OH^-] \quad (5.2)$$

where

$\lambda_1$	=	decay constant for dissolved phase [1/yr]
$[H^+]$	=	the hydrogen ion concentration [mole/l]
$[OH^-]$	=	the hydroxyl ion concentration [mole/l]

Note that  $[H^+]$  and  $[OH^-]$  can be computed from the pH of the aquifer using

$$[H^+] = 10^{-\text{pH}} \quad (5.3)$$

$$[OH^-] = 10^{-(14-\text{pH})} \quad (5.4)$$

For the case of sorbed phase hydrolysis, evidence suggests that base-neutralized hydrolysis can be neglected and that the acid-neutralized hydrolysis rate is enhanced by a factor of  $\alpha$ . Thus, the effective sorbed phase decay rate can be expressed as:

$$\lambda_2 = \alpha K_a^T [H^+] + K_n^T \quad (5.5)$$

where  $K_a$  = acid-catalyzed hydrolysis rate enhancement factor for sorbed phase with a typical value of 10.0, and  $\lambda_2$  = decay constant for the sorbed phase [1/yr].  $K_a^T$ ,  $K_b^T$  and  $K_n^T$  are chemical-specific constants.

### 5.1.2 Reference Temperature

The chemical-specific hydrolysis rates are specified for a constant reference temperature, the default value of which is 25°C.

### 5.1.3 Normalized Distribution Coefficient

The normalized distribution coefficient for organic carbon ( $k_{oc}$ ) is used in conjunction with the fractional organic carbon content to obtain the distribution coefficient ( $k_d$ ). The  $k_{oc}$  is a chemical-specific variable which is input as a constant. The use of  $k_{oc}$  to estimate sorption is appropriate for organic compounds which tend to sorb preferentially on the natural organic matter in the soil or aquifer.

### 5.1.4 Constituent Drinking Water Standard

Two additional parameters must be specified if a finite source simulation is being performed. These are: (1) the applicable drinking water standard for each constituent in the waste, and (2) the exposure averaging period used in the risk calculations for determining the drinking water standard. Usual values of the latter parameter are 70 years (lifetime exposure) or 30 years (average residence time). Note that the drinking water standard must be expressed in the same units used for the leaching concentration, usually mg/L. Both these parameters are entered as constants. By default, the exposure period for averaging the receptor well concentration is set to zero; in other words, the model calculates the peak receptor well concentration.

## 5.2 METALS

The sorption behavior of metals is divided into two groups. Those with linear sorption behavior and those with nonlinear sorption. The sorption characteristics of the first group is represented by a linear adsorption isotherm coefficient ( $k_d$ ) which is a function of the pH in the unsaturated zone. The relationship with the pH is described in the EPACMTP background document for Metals (EPA, 1996d). Metals that belong to this group are: As, Sb, Cr<sup>+6</sup>, Se, and Tl.

The sorption behavior of the second group is characterized by nonlinear sorption isotherms. Metals in this group are: Ba<sup>2+</sup>, Cd<sup>2+</sup>, Be<sup>2+</sup>, Cr<sup>3+</sup>, Ni<sup>2+</sup>, Pb<sup>2+</sup>, Ag<sup>2+</sup>, Zn<sup>2+</sup>, V<sup>4+</sup>. The sorption isotherms for these metals are calculated by MINTEQA2, a metal speciation model, and are provided to EPACMTP in tabular form as a secondary input file. The sorption isotherm data account for the effect of varying geochemical conditions in the soil and in the aquifer on the mobility of metal species by using different effective sorption isotherms which depend on a number of environmental master variables. These controlling master variables are listed in Table 5.2. For Monte Carlo analyses modeling, these parameters are treated as random variables. Sorption isotherms data are available for various combination of master variables varying from “low”, “medium”, or “high” values. This procedure is discussed in detail in the metals background document (EPA, 1996b). Probability distributions for the master variables are discussed below.

### 5.2.1 Soil and Aquifer pH

The pH distribution was obtained by analysis of nearly 25,000 field measured pH values obtained from EPA's STORET database. The data are represented by an empirical distribution with low and high values of 3.2 and 9.7, respectively and a median value of 6.8 (Table 5.3). The 0th and 100th percentile

values, determined from national distribution of pH, are lower and upper bounds of pH measurements. This distribution was derived from a literature search for reported pH values of uncontaminated groundwater. For modeling purposes it is assumed that the unsaturated zone and the saturated zone have the same pH value.

### 5.2.2 Fraction Iron-Hydroxide Adsorbent

Amorphous iron hydroxides (FeOx) represents one of the dominant adsorbents for metal sorption. Limited available data on iron hydroxide content is used to define a uniform distribution which results in a low value of 0.0126 and a high value of 1.115 percent iron hydroxide by weight. The values are obtained from analyses by Loux et al. (1990) on aquifer samples collected by the U.S. EPA Office of Solid Waste (OSW) in Florida, New Jersey, Oregon, Texas, Utah, and Wisconsin.

### 5.2.3 Leachate Organic Matter

The model uses a uniform distribution for the concentration of anthropogenic dissolved organic carbon (DOC<sub>a</sub>) in the leachate. The distribution has a low value of 0.001173 mg/L, and a high value of 0.00878 mg/L. The mixture of organic compounds used to represent the leachate-derived anthropogenic dissolved organic carbon is based on analyses of leachate samples collected by the OSW in Florida, New Jersey, Oregon, Texas, Utah, and Wisconsin (Loux et al., 1990).

### 5.2.4 Natural Organic Matter

The distribution for the unsaturated zone natural organic matter varies with soil type, and is specified as the percent organic matter. Conversely, the natural organic matter in the saturated zone is specified as the fraction organic carbon ( $f_{oc}$ ). The saturated zone fraction organic carbon has a Johnson SB distribution with mean and standard deviation (in arithmetic space) of  $4.32 \times 10^{-4}$  and 0.0456, respectively, and an upper bound of 0.0638. The percent organic matter and fraction organic carbon can be converted to fraction of organic carbon using:

$$\% OM = f_{oc} \times 174 \quad (5.6)$$

where the conversion factor of 174 is the reciprocal of the average mass fraction of carbon in organic matter (Enfield et al, 1982).

Table 5.2 Metals-Specific Variable and Default Distribution Types.

<b>Variable</b>	<b>Units</b>	<b>Distribution Code*</b>	<b>Default Distribution</b>
Metal Identification Number	---	0	Constant
Soil and aquifer pH		6	Empirical (Table 5.3)
Fraction Iron-Hydroxide absorbent	Weight fraction	4	Uniform
Leachate organic matter content	mg/l	4	Uniform
Natural organic matter	Weight fraction	7	Johnson SB
Fraction organic carbon	Weight fraction	7	Johnson SB

\* See Table 3.1

Table 5.3 Probability distribution of soil and aquifer pH.

<b>Cumulative Probability (percent)</b>	<b>pH Value</b>
0.0	3.20
1.0	3.60
5.0	4.50
10.0	5.20
25.0	6.07
50.0	6.80
75.0	7.40
90.0	7.90
95.0	8.20
99.0	8.95
100.0	9.70

**PART 3**

**SUBSURFACE FATE AND TRANSPORT SIMULATION**

## 6.0 UNSATURATED ZONE SIMULATION

A schematic view of the one-dimensional system simulated by the unsaturated zone module is provided in Figure 6.1.

Details on the mathematical formulation and solution techniques of the unsaturated zone flow and transport module are provided in the EPACMTP background document (EPA, 1996b). To guide the user in evaluating appropriate fate and transport options to simulate the processes in the subsurface, a summary of major assumptions is provided here:

- Flow of the fluid phase is isothermal and is governed by Darcy's law.
- Flow is one-dimensional, vertically downward, and at steady-state.
- The fluid is slightly compressible and homogeneous.
- The dynamics of a second phase (e.g., air or nonaqueous liquid) can be disregarded.

The solutions for transient and steady-state transport in the unsaturated zone are based on the following assumptions.

- The leachate concentration entering the soil is either constant (with a finite or infinite duration) or decreasing with time following a first-order decay process.
- Sorption of contaminants onto the soil solid phase is described by a linear or nonlinear (Freundlich) equilibrium isotherm.

In order to simulate flow and transport in the unsaturated zone between the base of the disposal facility and water table, the following data are required:

- Thickness of the unsaturated zone (depth to water table from base of disposal unit).
- Soil hydraulic parameters. If these parameters are not available, but the soil type is known, the parameter values from the database of Carsel and Parrish (1988) can be used. These data are used for Monte Carlo simulations.
- The water flow rate (infiltration rate) through the disposal unit. This input can be determined for landfills from the long term net percolation rate (precipitation minus runoff minus evapotranspiration). For surface impoundments, it may be determined from the depth of water ponding in the impoundment, and thickness and saturated conductivity of the impoundment liner. The code can derive the infiltration rate from these parameters.
- Soil transport parameters. If not available, the dispersivity can be estimated from the unsaturated zone thickness, and the retardation and decay coefficients can be estimated from the soil bulk density, fraction of organic matter and chemical-specific properties. Procedures for calculating these parameters are presented in the next five sections.

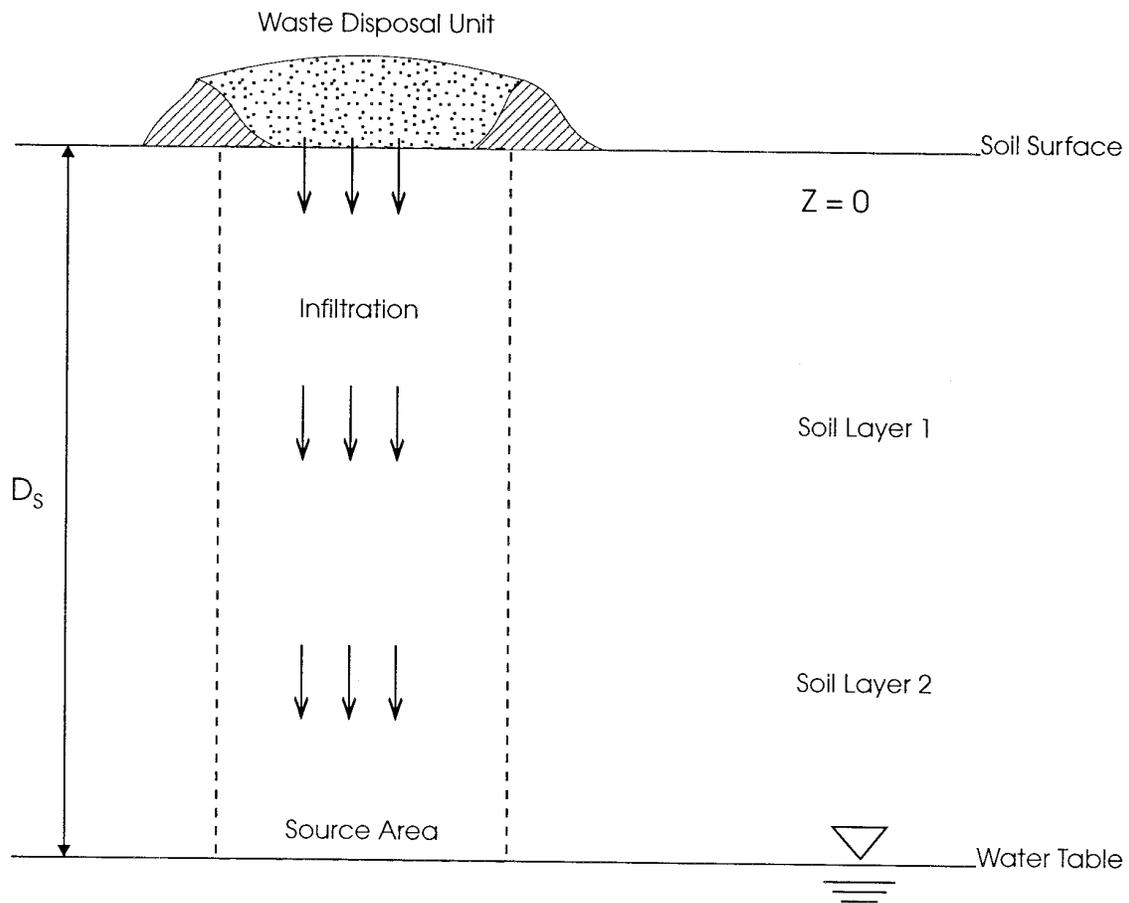


Figure 6.1 Cross-sectional view of the unsaturated zone considered by EPACMTP.

- The leachate concentration emanating from the base of the waste site. If a finite source is being simulated, the duration of the pulse must be specified. It is derived for landfills.
- The number of component species and decay reaction stoichiometry, in the case of chain decay reactions.
- Organic carbon partition coefficient ( $K_{oc}$ ) for organic chemicals and the effective partition coefficient ( $k_d$ ), as a function of concentration, in the case of metals with nonlinear sorption.

A list of unsaturated zone parameters is provided in Table 6.1.

## 6.1 THICKNESS OF THE UNSATURATED ZONE

The unsaturated zone thickness, or depth to the water table for each waste site is obtained from the regional hydrogeologic data base. Based on a site's location, the corresponding hydrogeologic region is selected. The unsaturated zone thickness is then selected randomly from data available for that hydrogeologic region. The frequency distribution of unsaturated zone thickness is in Appendix B.

## 6.2 SOIL CHARACTERISTIC CURVE PARAMETERS

Solution of the unsaturated zone flow requires knowledge of the soil characteristic curves, i.e., the relationship between water saturation and pressure head and between hydraulic conductivity and water saturation. The van Genuchten (1980) model is widely used for predicting soil-water content as a function of pressure head. Probability distributions for the parameters of this model were presented by Carsel and Parrish (1988). The variables analyzed by Carsel and Parrish include saturated hydraulic conductivity ( $K_s$ ), residual water content ( $\theta_r$ ), saturated water content ( $\theta_s$ ), and two empirical constants ( $\alpha$  and  $\beta$ ). The statistical parameters presented by Carsel and Parrish (1988) for three soil types used by EPA for Monte Carlo simulations are presented in Table 6.2. The frequency distribution of the saturated hydraulic conductivity, residual water content, and van Genuchten soil parameters ( $\alpha$  and  $\beta$ ) are also presented in Appendix B.

## 6.3 LONGITUDINAL DISPERSIVITY

The longitudinal dispersivity of the soil can be input as a distribution or it may be derived. If derived, it is computed as a linear function of the total depth of the unsaturated zone using

$$\alpha_{Lu} = 0.02 + 0.022 D_u \quad (6.1)$$

where:

$D_u$  = total depth of the unsaturated zone [m]

$\alpha_{Lu}$  = longitudinal dispersivity [m]

Equation (6.1) is based on a regression analysis of data presented by Gelhar et al. (1985), which are provided in Table 6.3. The correlation coefficient squared ( $R^2$ ) of equation (6.1) is 66 percent.

Table 6.1 Unsaturated Zone Specific Variables and Default Distribution Types.

	<b>Variable</b>	<b>Units</b>	<b>Distribution Code*</b>	<b>Default Distribution</b>
SATK	Saturated hydraulic conductivity ( $K_s$ )	cm/hr	2	Lognormal (Depends on soil type, Table 6.2)
ALPHA	Moisture retention parameter, $\alpha$	cm <sup>-1</sup>	2	Lognormal
BETA	Moisture retention parameter ( $\beta$ )		7	Johnson SB
WCR	Residual water content ( $\theta_r$ )		7	Johnson SB
WCS	Saturated water content ( $\theta_s$ )		0	Constant for each soil type
DSOIL	Thickness of unsaturated zone	m	99	Regional Site-based
DSPR	Dispersivity ( $\alpha$ )	m	-1	Derived based on regression analysis of data by Gelhar et al.
POM	Percent organic matter (% OM)		7	Johnson SB
RHOB	Bulk density ( $\rho_b$ )	g/cm <sup>3</sup>	0	Constant (1.65)
UFCOF	Freundlich sorption coefficient ( $K_f$ )	cm <sup>3</sup> /gr	-1	Derived from % OM and chemical-specific $K_{oc}$
UFEXP	Freundlich exponent ( $\eta$ )		0	Constant (1.0)
UCLAM	Chemical degradation rate coefficient ( $\lambda_{cu}$ )	1/yr	-1	Derived from chemical-specific hydrolysis constants
BIOU	Biological degradation rate coefficient ( $\lambda_{bu}$ )	1/yr	0	Constant (0.0)

\* See Table 3.1

Table 6.2 Statistical parameters for soil properties for three soil types (Carsel and Parrish, 1988). All values are in arithmetic space.

Variable	Distribution Type	Limits of Variation		Mean	Standard Deviation
		Minimum	Maximum		
<u>Soil Type - Silty Clay Loam</u>					
KS cm/hr	SB	0.	3.5	0.017	2.921
$\theta_r$	NO	0.00	0.115	0.089	0.0094
$\alpha$ cm <sup>-1</sup>	SB	0.00	0.15	.009	.097
$\beta$	NO	1.0	1.5	1.236	0.061
% OM	SB	0.0	8.35	0.11	5.91
$\rho_b$	Constant	-	-	1.67	-
$\theta_s$	Constant	-	-	0.43	-
<u>Soil Type - Silt Loam</u>					
KS cm/hr	LN	0.	15.0	.343	.989
$\theta_r$	SB	0.00	0.11	.068	0.071
$\alpha$ cm <sup>-1</sup>	LN	0.00	0.15	.019	0.012
$\beta$	SB	1.0	2.0	1.409	1.629
% OM	SB	0.0	8.51	0.105	5.88
$\rho_b$	Constant	-	-	1.65	-
$\theta_s$	Constant	-	-	0.45	-
<u>Soil Type - Sandy Loam</u>					
KS cm/hr	SB	0.	30.0	2.296	24.65
$\theta_r$	SB	0.	0.11	0.065	0.074
$\alpha$ cm <sup>-1</sup>	SB	0.	0.25	0.070	0.171
$\beta$	LN	1.35	3.00	1.891	0.155
% OM	SB	0.0	11.0	0.074	7.86
$\rho_b$	Constant	-	-	1.60	-
$\theta_s$	Constant	-	-	0.41	-

% OM = Percent Organic Matter  
 NO = Normal distribution  
 SB = Log ratio distribution,  $Y = \ln [(x-A)/(B-x)]$ ,  $A < x < B$   
 LN = Log normal distribution,  $Y = \ln[x]$   
 where Y = normal distributed parameter  
 x = actual data

Table 6.3      Compilation of field dispersivity values (Gelhar et al. 1985).

<b>Author</b>	<b>Type of Experiment</b>	<b>Vertical Scale of Experiment (m)</b>	<b>Longitudinal Dispersivity <math>\alpha_L</math> (m)</b>
Yule and Gardner (1978)	Laboratory	0.23	0.0022
Hildebrand and Himmelblau (1977)	Laboratory	0.79	0.0018
Kirda et al. (1973)	Laboratory	0.60	0.004
Gaudet et al. (1977)	Laboratory	0.94	0.01
Brissaud et al. (1983)	Field	1.00	0.0011, 0.002
Warrick et al. (1971)	Field	1.20	0.027
Van de Pol et al. (1977)	Field	1.50	0.0941
Biggar and Nielsen (1976)	Field	1.83	0.05
Kies (1981)	Field	2.00	0.168
Jury et al. (1982)	Field	2.00	0.0945
Andersen et al. (1968)	Field	20.00	0.70
Oakes (1977)	Field	20.00	0.20

## 6.4 FREUNDLICH SORPTION COEFFICIENT (DISTRIBUTION COEFFICIENT)

For organic compounds, the user must specify two isotherm parameters: the Freundlich sorption coefficient and the Freundlich exponent. A special case occurs when the isotherm is linear. In this case, the Freundlich exponent is 1.0. When the isotherm is linear, the leading Freundlich coefficient is known as the solid-liquid phase distribution coefficient ( $k_d$ ). The distribution coefficient may be specified directly or as a derived parameter. In the latter case, it is computed from the fraction organic carbon and the organic carbon partition coefficient ( $k_{oc}$ ), the latter of which must be given in the chemical-specific input group. For metals, this input parameter is not used, instead the  $k_d$  is calculated either as a function of pH, or is provided in tabular form as a function of the concentration value (EPA, 1996c).

## 6.5 PERCENT ORGANIC MATTER

The soil bulk density and the organic matter content for the three soil types are included in Table 6.2. These values are based on the nationwide data base developed by Carsel and Parrish (1988). The percent organic matter is converted by EPACMTP to fractional organic carbon content through the following equation (Enfield et al., 1982):

$$f_{oc} = \frac{\%OM}{174} \quad (6.2)$$

where:

$f_{oc}$  = fractional organic carbon content,  
 $\%OM$  = percent organic matter, and  
174 = conversion factor.

Once the fractional organic carbon content is obtained, the linear distribution coefficient can be found using:

$$k_d = k_{oc} f_{oc} \quad (6.3)$$

where:

$k_d$  = distribution coefficient [ $\text{cm}^3/\text{g}$ ], and  
 $k_{oc}$  = normalized organic carbon distribution coefficient [ $\text{cm}^3/\text{g}$ ].

Note that equation (6.3) is based on the assumption that hydrophobic binding dominates the sorption process (Karickhoff, 1985). The frequency distribution of percent organic matter in the soil is in Appendix C.

## 6.6 FREUNDLICH ISOTHERM EXPONENT

For a nonlinear isotherm, the Freundlich exponent for each chemical species must be provided in addition to the distribution coefficient. The nonlinear isotherm is currently handled within MINTEQA2 isotherm data. If this parameter is omitted from the data file, it is assigned a default value of 1.0, which is equivalent to specifying a linear sorption isotherm. In the case of metal transport simulation, tabulated values of  $k_d$  versus concentration are read in from an external data file, and the Freundlich isotherm parameters are not used.

## 6.7 CHEMICAL AND BIOLOGICAL TRANSFORMATION COEFFICIENTS

EPACMTP accounts for biochemical transformation processes using a lumped first-order decay coefficient. The overall decay coefficient is the sum of the chemical and biological transformation coefficients.

$$\lambda_u = \lambda_{cu} + \lambda_{bu} \quad (6.4)$$

where

$\lambda_u$  = overall decay coefficient (first-order transformation) (1/yr)

$\lambda_{cu}$  = transformation coefficient due to chemical transformation (1/yr)

$\lambda_{bu}$  = transformation coefficient due to biological transformation (1/yr)

The coefficients  $\lambda_{cu}$  and  $\lambda_{bu}$  are specified in the EPACMTP data input file, either as constants or as a distribution. By default,  $\lambda_{bu}$  is set to zero and  $\lambda_{cu}$  is a derived parameter, in which case it is calculated from the chemical-specific hydrolysis constants:

$$\lambda_{cu} = \frac{\lambda_1 \phi + \lambda_2 \rho_b k_d}{\phi + \rho_b k_d} \quad (6.5)$$

where

$\lambda_1$  = hydrolysis constant for dissolved phase [1/yr],

$\lambda_2$  = hydrolysis constant for sorbed phase [1/yr],

$\rho_b$  = bulk density of the porous media [g/cm<sup>3</sup>], and

$\phi$  = porosity [cm<sup>3</sup>/cm<sup>3</sup>].

Note that  $\lambda_1$  and  $\lambda_2$  may be temperature and pH dependent. The values of temperature and pH for the unsaturated zone are considered to be the same as those generated for the saturated zone (see Sections 7.10 and 7.11).

## 7.0 SATURATED-ZONE SIMULATION

The aquifer system simulated by the saturated-zone module of EPACMTP is depicted schematically in Figure 7.1. Note that the system is assumed to be symmetric in the horizontal-transverse direction about the plane  $y = 0$ ; thus only one-half of the system along the positive  $y$ -axis is simulated by the model. The vertical coordinate ( $z$ ) is taken to be positive downward with  $z=0.0$  at the water table. The shaded area on top of the aquifer represents the area directly underneath the waste site. Contaminants entering the water table are assumed to be distributed uniformly over this area.

Groundwater flow in the saturated zone is simulated using a steady-state solution for predicting hydraulic head and Darcy velocities in a constant thickness groundwater system subject to infiltration and recharge along the top of the aquifer and a regional (ambient) gradient defined by upstream and downstream head boundary conditions.

As illustrated in Figure 7.1, EPACMTP simulates a portion of the aquifer with length and width  $x_L$  and  $\frac{1}{2} y_L$ , respectively. The modeled aquifer region encompasses the waste site as well as any specified observation wells. The value of  $x_L$  and  $y_L$  are determined internally by EPACMTP, based upon specified input parameters (disposal unit area, receptor well distance, dispersivity) of the simulated problem. The  $x_L$  and  $y_L$  are determined to be large enough that boundary effects will be negligible. The boundary-head values  $H_1$  and  $H_2$  are in turn determined from the regional hydraulic gradient,  $r$ , and the selected aquifer length,  $x_L$ :

$$\begin{aligned} H_1 &= rx_L \\ H_2 &= 0 \end{aligned} \tag{7.1}$$

If necessary, the regional gradient is computed from the longitudinal saturated hydraulic conductivity,  $K_x$ , and the regional ambient groundwater flow rate per unit area,  $q$ :

$$r = q/K_x \tag{7.2}$$

The solution for groundwater flow is based on the following assumptions:

- The aquifer is homogeneous.
- Groundwater flow is steady.
- The saturated thickness of the aquifer remains constant and mounding is represented by the head distribution on the top boundary.
- Flow is isothermal and governed by Darcy's law.
- The fluid is slightly compressible and homogeneous.



In addition to modeling fully three-dimensional (3D) groundwater flow and contaminant fate and transport, EPACMTP offers the option to perform an efficient 2D modeling approximation. When this option is selected, the model ignores either the flow component in the horizontal-transverse (-y) direction, or the flow component in the vertical (-z) direction. The appropriate 2D approximation is selected automatically by the code, based on the relative magnitude of plume movement in the horizontal-transverse versus the vertical direction. Details of this procedure are provided in the saturated zone background document (EPA, 1996b).

The saturated zone transport module describes the advective-dispersive transport of dissolved contaminants in a three-dimensional, constant thickness aquifer. The initial contaminant concentration is set to zero. The concentration gradient along the downstream boundary is zero, and the lower aquifer boundary is taken to be impermeable. A zero concentration condition is used for the upstream aquifer boundary. Contaminants enter the saturated zone through a patch source of either constant concentration or constant mass flux on the upper aquifer boundary. The source may be of finite or infinite duration. Recharge of contaminant-free infiltration water occurs along the upper aquifer boundary outside the patch source. Transport mechanisms considered are advection, dispersion, linear or nonlinear equilibrium adsorption, and first-order decay with daughter product formation. As in the unsaturated zone, the saturated zone transport module can simulate multi-species transport involving chained-decay reactions. The saturated zone transport module of EPACMTP can perform either a fully three-dimensional transport simulation, or provide a 2D approximation. The latter approach ignores advection in either the horizontal transverse (-y) direction, or the vertical (-z) direction. In the course of a Monte Carlo simulation, the appropriate 2D approximations are selected automatically for each individual Monte Carlo iteration.

The major simplifying assumptions used to simulate contaminant transport in the saturated zone are:

- The flow field is at steady state.
- The aquifer is homogeneous and initially contaminant free.
- Adsorption onto the solid phase is described by a linear or nonlinear equilibrium isotherm.
- Chemical and/or biochemical degradation of the contaminant can be described as a first-order process.
- For a multicomponent decay chain, the number of component species (parent and daughters) does not exceed seven.
- The mass flux of contaminants through the source is either constant or controlled by first-order decay, until all mass has been released from the source.
- The chemical is dilute and present in the aqueous and aquifer solid phases only.

EPACMTP variables for saturated zone are listed in Table 7.1. Some of these parameters can be input directly or can be computed by the code using the relationships shown in subsequent sections. If a multi-species simulation is desired, the chemical-dependent parameters (e.g. decay coefficient, Freundlich parameters) must be repeated for each of the NSPECI components in the decay chain.

A number of the parameters are characterized by nationwide distributions. However, the key hydrogeological parameters: hydraulic conductivity, hydraulic gradient, saturated thickness, and depth to water table and groundwater temperature, are defined by regional distributions obtained from the API's Hydrogeologic Data base for Modeling (HGDB, Newell et al., 1990). The procedure for determining these parameters is as follows: The HGDB contains data on depth to groundwater, hydraulic conductivity, hydraulic gradient, and saturated thickness for approximately 400 hazardous waste sites nationwide. Each site is also classified in terms of 12 hydrogeological regions, see Table 7.2. This classification is based on the USGS groundwater resources classification (USGS, 1984). As a result, data are available for the above mentioned key hydrogeological parameters for each of the 12 hydrogeological environments.

Based on the locations of each of the waste management units in the EPACMTP modeling database (see source-specific parameters), the hydrogeologic environment for each unit was determined using USGS state-by-state water resource maps (USGS, 1984). Note that EPACMTP uses a total 13 hydrogeological environments (Table 7.2). The hydrogeological environment no. 13 is assigned to those waste sites for which no specific hydrogeological environment could be identified from the state-by-state USGS groundwater maps. The aquifer parameters for this 13th environment are the mean values from the entire HGDB database. In other words, if a waste site is not classifiable in terms of the hydrogeological environment, it is assigned nationwide average values for hydraulic conductivity, depth to groundwater, saturated thickness and hydraulic gradient.

During each iteration of the Monte Carlo analysis, a waste unit is first selected at random (e.g., from the OPPI set of waste sites). This also determines the climatic and hydrogeologic environment and, therefore, the distribution of the key hydrogeologic parameters. It should be noted that for each hydrogeologic environment, the correlations between the hydrogeologic parameters (which represent measurements taken at the same region) are preserved in the analysis. This is done by selecting the HGDB parameters together. For instance, assume that for hydrogeologic environment A, there are 20 sets of hydrogeologic parameters, i.e. combinations of unsaturated zone depth, hydraulic conductivity, hydraulic gradient, and saturated thickness measured at 20 locations that fall in that hydrogeologic environment. The aquifer parameter values used in each model run for waste sites located in hydrogeologic environment A are assigned by randomly selecting one out of the 20 parameter combinations.

If data for one or more parameters in the selected set are missing, they are generated based on the statistical correlations among the parameters for that hydrogeological environment. As a result, regional differences in aquifer characteristics as well as dependencies between hydrogeological parameters are automatically accounted for in the EPACMTP Monte Carlo analysis.

Table 7.1 Aquifer-Specific Variables and Default Distribution Types.

Variable	Units	Distribution Code*	Default Distribution
Particle diameter (d)	(cm)	6	Empirical (Table 6.12)
Porosity ( $\phi$ )		-1	Derived from d
Bulk density ( $\rho_b$ )	g/cm <sup>3</sup>	-1	Derived from
Aquifer thickness (B)	m	99	Regional Site-based
Hydraulic conductivity (K)	m/y	99	Regional Site-based
Hydraulic gradient (S)		99	Regional Site-based
Seepage velocity (V)	m/y	-1	Derived from K, S, $\phi$
Retardation factor ( $R_s$ )		-1	Derived from $k_d$ , $\phi$ , and $\rho_b$
Longitudinal dispersivity ( $\alpha_L$ )	m	8	Empirical (Table 6.14)
Transverse dispersivity ( $\alpha_T$ )	m	8	Empirical
Vertical dispersivity ( $\alpha_v$ )	m	8	Empirical
Temperature (T)	°C	99	Regional Site-based (Figure 6.2)
pH		6	Empirical
Fractional organic carbon content ( $f_{oc}$ )		7	Johnson - SB
Radial distance of observation well	m	6	Empirical (Table)
Angle off-center		4	Uniform (0-90°) from plume centerline
Depth of well below water table		4	Uniform (Fraction of saturated zone thickness)
Decay coefficient ( $\lambda_u$ )	1/y	-1	Derived from T, pH, $\rho_b$ , $\phi$
Leading Freundlich sorption coefficient ( $k_d$ )	cm <sup>3</sup> /gr	-1	Derived from $k_{oc}$ , $f_{oc}$
Freundlich isotherm exponent ( $\eta$ )		0	Constant (=1.0)
Diffusion coefficient	m <sup>2</sup> /y	0	Constant (=0.0)
Anisotropy ratio ( $K_x/K_z$ )		0	Constant (=1.0)

\* See Table 3.1

Table 7.2 Regional Hydrogeologic Environments.

Region	Description
1	Metamorphic and Igneous
2	Bedded Sedimentary Rock
3	Till Over Sedimentary Rock
4	Sand and Gravel
5	Alluvial Basins Valleys and Fans
6	River Valleys and Floodplains with Overbank Deposits
7	River Valleys and Floodplains without Overbank Deposit
8	Outwash
9	Till and Till Over Outwash
10	Unconsolidated and Semiconsolidated Shallow Aquifers
11	Coastal Beaches
12	Solution Limestone
13	Others (unclassified Hydrogeological Environments)

## 7.1 PARTICLE DIAMETER

For Monte Carlo analyses, porosity and bulk density are determined from the mean particle diameter. The mean particle diameter distribution is based on data compiled by Shea (1974). Shea (1974) presents a frequency distribution of particle sizes based on analysis of 11,000 samples. These data have been adopted for nationwide modeling purposes, using particle sizes ranging from a lower bound of  $4 \times 10^{-4}$  cm to an upper bound of 0.8 cm. The resulting empirical distribution is presented in Table 7.3. The frequency distribution of particle diameter of the aquifer is provided in Appendix C.

Alternatively, if the particle diameter is treated as a derived parameter, then its value is calculated using the value of porosity (which may be constant or randomly generated from a probability distribution) using an empirical relationship based on data reported by Davis (1969):

$$d = \exp [(0.261 - \phi)/0.0385] \quad (7.3)$$

where:

$d$  = mean particle diameter [cm]

$\phi$  = porosity [dimensionless]

## 7.2 POROSITY

In the absence of a user-specified distribution for porosity, porosity can be calculated from the particle diameter by rewriting (7.3):

$$\phi = 0.261 - 0.0385 \ln(d) \quad (7.4)$$

where  $\phi$  and  $d$  are defined in Section 7.1.

This approximation yields the total porosity of the aquifer. For contaminant transport assessments, it is more appropriate to use effective porosity,  $\phi_e$ , than total porosity. The effective porosity can be significantly smaller than the total porosity, although an exact relationship cannot be established. Mcworter and Sunada (1977) present data on total and effective porosity for a range of aquifer materials. Their data were used to establish ranges for the ratio between effective and total porosity as a function of grain size (Table 7.4). For Monte Carlo assessments, it is assumed that the actual ratio varies uniformly between the upper and lower value for  $\phi_e/\phi$  in each particle-size class. For a given value of the mean aquifer grain size, the total porosity can thus be converted into an effective porosity. Overall lower and upper bounds of 0.05 and 0.50 are imposed on the effective porosity. It should be noted that EPACMTP makes the conversion from total to effective porosity only if porosity is specified as a derived parameter (porosity is calculated from grain size), which is the default option of the model. In all other cases, no conversion is performed and the user must specify the actual porosity data to be used by the model, providing a distribution for either total porosity or effective porosity directly.

Table 7.3 Empirical distribution of mean particle diameter (based on Shea, 1974).

<b>Particle Diameter (cm)</b>	<b>Cumulative Probability</b>
3.9 10 <sup>-4</sup>	0.000
7.8 10 <sup>-4</sup>	0.038
1.6 10 <sup>-3</sup>	0.104
3.1 10 <sup>-3</sup>	0.171
6.3 10 <sup>-3</sup>	0.262
1.25 10 <sup>-2</sup>	0.371
2.5 10 <sup>-2</sup>	0.560
5.0 10 <sup>-2</sup>	0.792
1.0 10 <sup>-1</sup>	0.904
2.0 10 <sup>-1</sup>	0.944
4.0 10 <sup>-1</sup>	0.976
8.0 10 <sup>-1</sup>	1.000

Table 7.4 Ratio between effective and total porosity as a function of particle diameter (after McWorter and Sunada, 1977).

Mean Particle Diameter (cm)	$\phi_e/\phi$ Range
$\leq 6.25 \cdot 10^{-3}$	0.03 - 0.77
$6.25 \cdot 10^{-3} - 2.5 \cdot 10^{-2}$	0.04 - 0.87
$2.5 \cdot 10^{-2} - 5.0 \cdot 10^{-2}$	0.31 - 0.91
$5.0 \cdot 10^{-2} - 1.0 \cdot 10^{-1}$	0.58 - 0.94
$> 1.0 \cdot 10^{-1}$	0.52 - 0.95

### 7.3 BULK DENSITY

The aquifer bulk density directly influences the retardation of solutes and is related to aquifer porosity. An exact relationship between porosity, particle density, and the bulk density can be derived (Freeze and Cherry, 1979). Assuming the particle density to be 2.65 g/cm<sup>3</sup>, this relationship can be expressed as:

$$\rho_b = 2.65(1 - \phi) \quad (7.5)$$

where  $\rho_b$  is the bulk density of the soil [g/cm<sup>3</sup>].

### 7.4 AQUIFER THICKNESS

The aquifer saturated thickness is assigned as a regional site-based parameter. The frequency distribution of aquifer thickness is shown in Appendix C.

### 7.5 HYDRAULIC CONDUCTIVITY

By default, the aquifer hydraulic conductivity is assigned as a regional site-based parameter using the procedure outlined at the beginning of this section. The frequency distribution of aquifer hydraulic conductivity is given in Appendix C.

Alternatively, the hydraulic conductivity can be specified as a derived parameter. In this case it is calculated directly from the particle diameter using the Kozeny-Carman (Bear, 1979) equation

$$K = \frac{\rho g}{\mu} \frac{\phi^3}{(1 - \phi)^2} \frac{d^2}{1.8} \quad (7.6)$$

where:

- $K$  = the hydraulic conductivity [cm/s]
- $\rho$  = the density of water [kg/m<sup>3</sup>]
- $g$  = acceleration due to gravity [m/s<sup>2</sup>]
- $\mu$  = the dynamic viscosity of water [N-s/m<sup>2</sup>]
- $d$  = particle diameter [m]

In Equation (7.6) the constant 1.8 includes a unit conversion factor to yield  $K$  in units of cm/s. Both the density and the dynamic viscosity of water are functions of temperature and are computed using the regression equations presented in CRC (1981). Note that the particle diameter,  $d$ , must be in units of meters, as opposed to centimeters as used in equation (7.3).

## 7.6 HYDRAULIC GRADIENT

The hydraulic gradient is assigned as a regional, site-based parameter using the procedure outlined in the beginning of this section. The frequency distribution of the hydraulic gradient is provided in Appendix C.

## 7.7 SEEPAGE VELOCITY

The seepage velocity is related to the aquifer properties through Darcy's law. The regional seepage velocity may be input directly or it may be a derived parameter (default). In the latter case, it is computed as

$$v_x = \frac{K_x}{\phi_e} r \quad (7.7)$$

where

- $v_x$  = regional seepage velocity in x-direction [m/y]
- $K_x$  = hydraulic conductivity in x-direction [m/y]
- $r$  = regional hydraulic gradient [m/m]
- $\phi_e$  = effective porosity [dimensionless]

Default lower and upper bounds for the seepage velocity are 0.1 and  $1.1 \times 10^4$  m/y, respectively. The range of seepage velocity values is based on survey data reported by Newell et al (1990).

## 7.8 RETARDATION FACTOR

The retardation factor is defined for a linear adsorption isotherm by

$$R_s = 1 + \frac{\rho_b k_d}{\phi} \quad (7.8)$$

where

- $\rho_b$  = bulk density of the porous media [ $\text{g}/\text{cm}^3$ ]
- $k_d$  = distribution coefficient [ $\text{cm}^3/\text{g}$ ]
- $\phi$  = porosity

When the sorption isotherm is nonlinear,  $R$  is no longer constant but depends on concentration (see Section 2.0). In this case,  $R$  must be given as a derived variable and the  $k_d$ -concentration relation must be specified by the user in terms of two Freundlich coefficients.

For the modeling of metals, a linear sorption isotherm is used for the saturated zone. The effective  $k_d$  value is determined from the maximum contaminant concentration at the water table and values of the four environmental master variables (pH, iron-oxide, leachate organic matter, and natural organic matter in the aquifer), following the procedure described in the metals background document (EPA, 1996b).

## 7.9 DISPERSION COEFFICIENTS

The spreading and dilution of the contaminant plume in the saturated zone is controlled by two mechanisms: advection and dispersion. EPACMTP allows for non-uniform groundwater flow due to vertical recharge and infiltration from the waste site. The model simulates actual spreading mechanisms occurring in the field. For non-degrading contaminants, the dilution caused by dispersive mixing is a controlling factor in determining the concentration observed at a receptor well. Somewhat surprisingly therefore is the fact, that in Monte Carlo analyses, transport is a relatively insensitive to dispersion. The reason for this is as follows: low dispersivities will lead to a compact, concentrated plume. If the plume is relatively small, the likelihood that the receptor well will intercept the plume is reduced, but the concentration in the well, if it does, will be high. High dispersivities will lead to a more dilute plume which occupies a greater volume, thereby increasing the likelihood that a receptor well will intercept the plume. Concentrations in the plume however, are likely to be lower than in the first case. In the course of a full Monte Carlo analysis, these effects will tend to compensate for each other.

The model computes the longitudinal, lateral, and vertical dispersion coefficients as the product of the seepage velocity and longitudinal ( $\alpha_L$ ), transverse ( $\alpha_T$ ) and vertical ( $\alpha_V$ ) dispersivities. A literature review indicated the absence of a generally accepted theory to describe dispersivities, although a strong dependence on scale has been noted (EPRI, 1985; Gelhar et al., 1992).

In the absence of user-specified values or distributions, the default model distribution is utilized if the distribution type of dispersivities is set equal to 8, which represents a probabilistic formulation for the longitudinal dispersivity as shown in Table 7.5 [Gelhar, 1986, Personal communication]. Within each of the three classes, the longitudinal dispersivity is assumed to be uniform. Note that the values of longitudinal dispersivity in Table 7.5 are based on a receptor well distance of 152.4 m. For distances other than 152.4 m, the following equation is used:

$$\alpha_L(x_i) = \alpha_L(x_i = 152.4)(x_i/152.4)^{0.5} \quad (7.9)$$

where  $x_i$  is the average horizontal travel distance defined as

$$x_i = \frac{1}{2}x_w + x_r \quad (7.10)$$

In other words, the travel distance  $x_i$  is equal to the distance of the receptor well ( $x_r$ ) from the downgradient facility boundary, plus one-half of the facility dimension. The average distance for all of the contaminants to migrate to the edge of the waste management unit is equal to one half the length of the unit or  $\frac{1}{2}x_w$ . The minimum value of  $\alpha_L$  is 0.01 m. The input mean value for  $\alpha_T$  and  $\alpha_V$  is the ratio of  $\alpha_L$  to  $\alpha_T$  and/or  $\alpha_V$ . Hence, the desired dispersivity is computed as the longitudinal dispersivity divided by the user-specified mean value. The values assigned to  $\alpha_T$  and  $\alpha_V$  are based on the relationship with  $\alpha_L$ . This option allows the user to define different values for the ratios of the longitudinal to the vertical and/or transverse dispersivities. By default, the following ratios are used:  $\alpha_L/\alpha_T = 8$  and  $\alpha_L/\alpha_V = 160$ . The frequency distribution of the aquifer longitudinal dispersivity is provided in Appendix C.

Table 7.5 Probabilistic representation of longitudinal dispersivity.

Cumulative Probability	$\alpha_L$ (m)*
0.0	0.1
0.1	1.0
0.7	10.0
1.0	100.0

\*Assumes  $x_t = 152.4$  m (see eq. 7.9)

The relationship in equation (7.9) has been derived based on an informal review of available data. More recently, Gelhar et al. (1992) have compiled and documented results from a large number of studies in which dispersivity values have been reported. These studies represent a wide range of spatial scales, from a few meters to over ten-thousand meters. The data as presented by Gelhar et al. (1992) show a clear correlation between scale and apparent dispersivity. The relationship (7.9) used in EPACMTP describes the observed data reasonably well. The field data suggest a somewhat steeper slope of the distance-dispersivity relation on a log-log scale than is used in the modeling analyses. A sensitivity analysis performed using EPACMTP (HydroGeoLogic, 1992) has shown that the model results are virtually identical when the slope is varied from 0.5 to 1.5. For this reason the original relationship as shown in (7.9) has been retained. The data presented by Gelhar et al. (1992) also show that the ratios between longitudinal, and horizontal and vertical transverse dispersivities used in the nationwide modeling, are consistent with published data.

## **7.10 TEMPERATURE**

Groundwater temperature is assigned as a regional parameter based on the location of the waste management unit. For each waste site, the assigned temperature is obtained from averaging the upper and lower temperatures within a region as shown in Figure 7.2.

## **7.11 GROUNDWATER pH**

A nationwide groundwater pH distribution was derived from EPA's STORET data base. The model assumes that the groundwater is sufficiently buffered such that pH is not influenced by the input of contaminants or changes in temperature. The default distribution is an empirical distribution (Table 5.3) with a median value of 6.8 and lower and upper bounds of 3.2 and 9.7, respectively.

## **7.12 FRACTIONAL ORGANIC CARBON CONTENT**

The organic carbon content,  $f_{oc}$ , is used to determine the linear distribution coefficient,  $k_d$ . This approach is valid for organic contaminants containing hydrophobic groups. These chemicals will tend to sorb preferentially on non-polar natural organic compounds in the soil or aquifer. Unfortunately, few if any comprehensive subsurface characterizations of organic carbon content exist. In general, the reported values are low, typically less than 0.01. A low range for  $f_{oc}$  was assumed and the distribution shape was based on the distribution of measured dissolved organic carbon recorded as entries to EPA's STORET data base. The default distribution for fractional organic carbon content is a Johnson SB distribution with a mean and standard deviation in arithmetic space of  $4.32 \times 10^{-4}$  and 0.0456, respectively and upper and lower limits of 0.064 and 0.0, respectively. In the case of metals, the sorption is controlled by complex geochemical interactions which are simulated using MINTEQA2 (EPA, 1996d).

## **7.13 RECEPTOR WELL LOCATION**

A receptor well is a hypothetical drinking water well that is located downgradient of the waste management unit in consideration. It represents the location at which the potential exposure to the groundwater is measured. A receptor well can be located 1) anywhere downgradient of the waste management unit, 2) within the areal extent of the contaminant plume, and/or 3) only along the contaminant plume centerline. The receptor well depth can be positioned anywhere within the saturated zone. The user specifies the receptor well location by assigning the following:

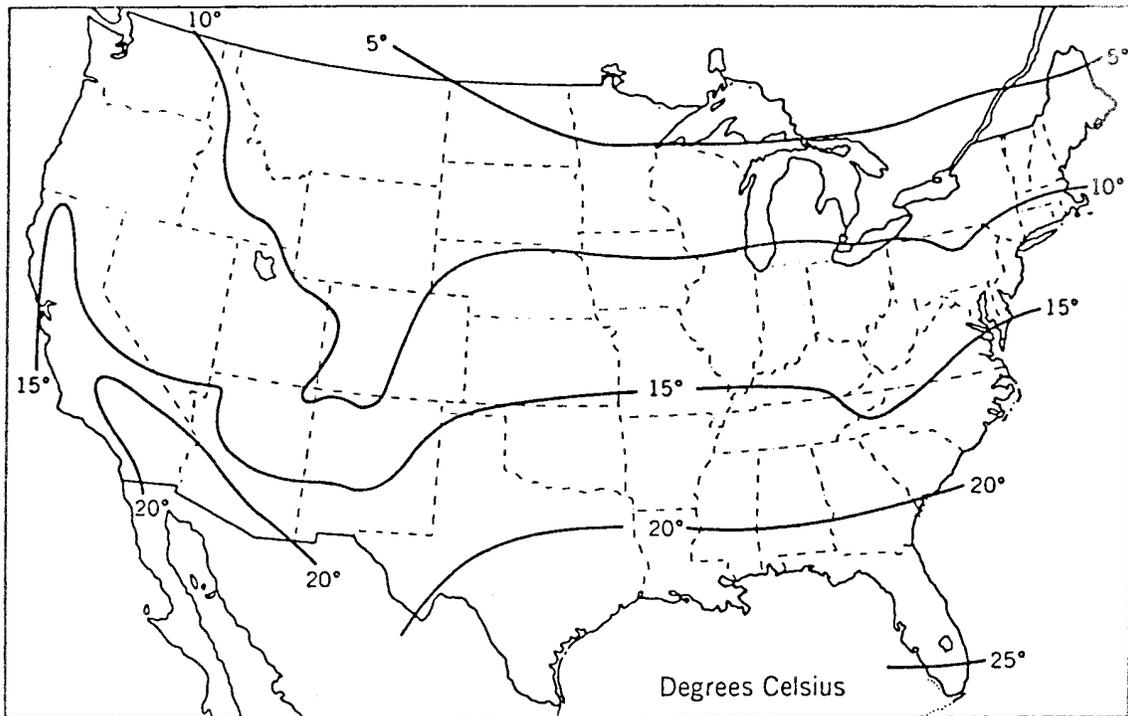


Figure 7.2 Groundwater temperature distribution for shallow aquifers in the United States. (After Collins, 1925)

- x, distance from the waste unit
- y, distance from the plume centerline
- z, well depth within the saturated zone

By default, the y-location of the receptor well is allowed to be anywhere downgradient from the waste source, i.e., the angle off-center varies between 0 and 90 degrees.

In a Monte Carlo simulation, the primary output from the model is the exposure concentration at receptor well located down gradient from the waste site, within a one-mile distance from the site. Available studies and surveys suggest that on average, multiple down-gradient wells are present within this one-mile distance. To ensure a degree of conservatism in the modeling analysis, the model computes the concentration at the *nearest* down gradient well. Information on the downstream distance to the nearest receptor well can be obtained from the OSW landfill survey (EPA, 1993). The data are presented as an empirical distribution in Table 7.6. At most waste sites included in this survey, the direction of ambient groundwater flow was in most cases not known exactly; it can therefore not be ascertained that the nearest receptor well is located directly along the plume centerline. To reflect uncertainties and variations in the location of the receptor well in relation to the direction of ambient groundwater flow, the modeled well is allowed to be positioned at a variable y-distance from the plume centerline. EPACMTP incorporates two options for determining the x- and y-coordinates of the receptor well.

The first, and default, option involves determining the x- and y-coordinates of the receptor well as a function of the radial distance, R, to the edge of the waste unit, and the angle off-center,  $\theta$ , as depicted in Figure 7.3a. In this case the x- and y-coordinate values must be specified as derived variables and are computed as

$$x_r = R \cos \theta \quad (7.11)$$

$$y_r = R \sin \theta \quad (7.12)$$

where

- R = radial distance between waste unit and well (m),
- $\theta$  = angle measured counter-clockwise from the plume centerline (degrees)
- $x_r, y_r$  = Cartesian coordinates of the receptor well (m)

To include all wells located downstream of the waste units, the angle  $\theta$  is taken to be uniformly distributed between 0 and 90°. R is determined using the empirical distribution shown in Table 6.15. Optionally, the y-coordinate of the well can be constrained to lie within the areal extent of the main contaminant plume as defined by

$$y_r \leq y_0 + 3[2\alpha_T(x_w + x_r)]^{1/2} \quad (7.13)$$

where

- $y_0$  = half-width of the waste unit in the y-direction (m)
- $x_w$  = length of the waste unit in the x-direction (m)
- $\alpha_T$  = horizontal transverse dispersivity (m)

This approximation for the lateral extent of the contaminant plume is based on the assumption that plume spreading in the horizontal-transverse direction is caused by dispersive mixing, which results in a Gaussian profile of the plume cross-section. Use of (7.13) implies that 99.7% of the contaminant mass will be present inside the transverse plume limit.

The shaded area in Figure 7.3a indicates the area occupied by the contaminant plume. The option to force the well location to lie within the areal plume boundaries is selected in EPACMTP by setting the logical control parameter LYCHK = TRUE in group GP02 of the data input file.

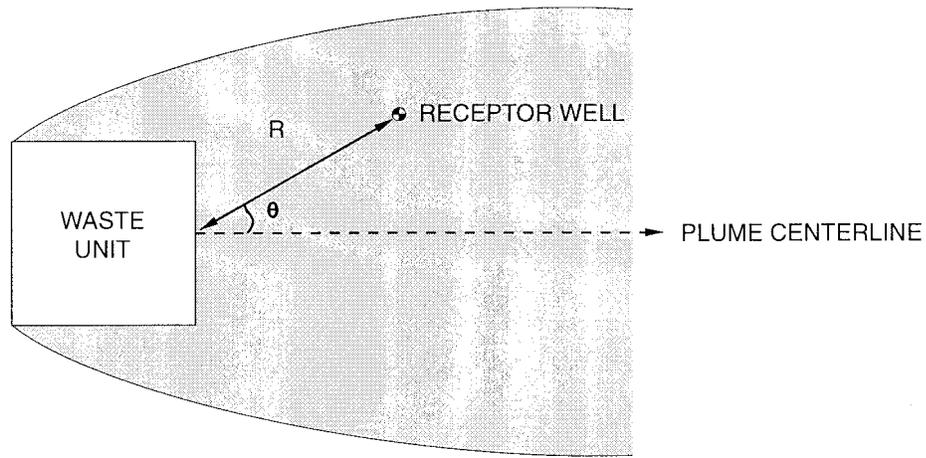
The second method imbedded in EPACMTP to determine the receptor well location is to generate a well position directly so that the well is located uniformly between the plume centerline and the areal plume boundary, for any given x-distance (Figure 7.3b). With this option, a x-distance is generated from the empirical distribution in Table 7.6. Next, the y-coordinate of the well is generated from a uniform distribution with a minimum value of zero, and a maximum value given by Equation (7.13). To select this option, the parameter LYCHK should be set to TRUE, the receptor well x-distance should be specified as an empirical parameter with values as given in Table 7.6, and the receptor well y-distance should be given as a uniform distribution. The frequency distributions of radial distance to the well and its off-center angle are provided in Appendix C.

Several options are available for specifying the vertical position of the well intake point below the water table. The first, and default, option is to model the vertical position of the well as being uniformly distributed between the water table ( $z=0$ ) and the saturated aquifer thickness. This option is selected by specifying the z-position as a uniform distribution with lower and upper limits of 0.0 and 1.0. EPACMTP will multiply this uniformly generated value by the saturated zone thickness to yield the actual receptor well depth below the water table for each Monte Carlo iteration.

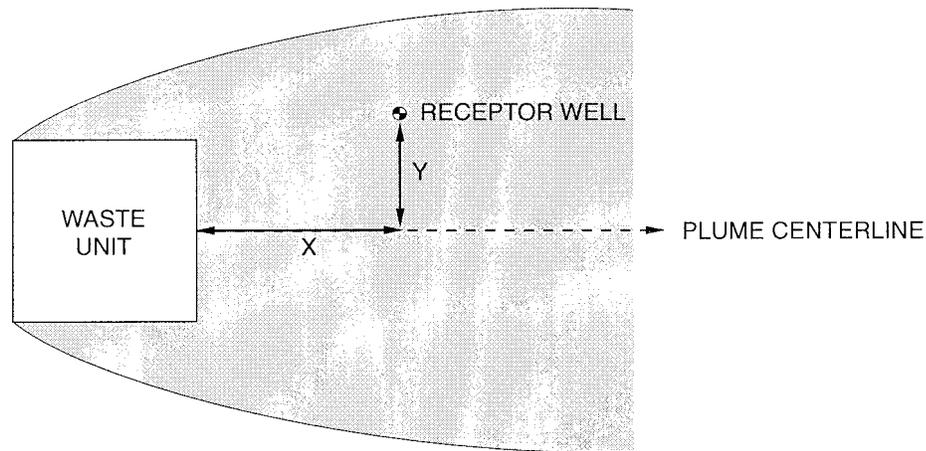
In the second option, data on the depth of receptor wells obtained from Agency surveys, can be used directly in the model as an empirical distribution. The data values range from 15 ft (4.5 m) to 301 ft (90.9 m). Table 7.7 shows the distribution of well depths and the corresponding cumulative probability values. When the generated value for the vertical position of the receptor well intake point exceeds the saturated thickness of the aquifer (a physically impossible condition), a new well position is generated to ensure that the well depth is always less than the saturated thickness. Conversely, the well depth cannot be less than the minimum depth to the saturated zone.

Table 7.6 Cumulative probability of distance to nearest receptor well for landfills (from EPA, 1993d).

Cumulative Probability	Distance (R) (m)
0.0	0.6
0.03	13.7
0.04	19.8
0.05	45.7
0.10	103.6
0.15	152.4
0.20	182.9
0.25	243.8
0.30	304.8
0.35	304.8
0.40	365.7
0.45	396.2
0.50	426.7
0.55	457.2
0.60	609.6
0.65	762.0
0.70	804.6
0.75	868.6
0.80	914.4
0.85	1158.2
0.90	1219.1
0.95	1371.5
0.98	1523.9
1.00	1609.3



(a)



(b)



Figure 7.3 Schematic plan view showing procedure for determining the downstream location of the receptor well: (a) well location determined using radial distance,  $R$ , and angle off center  $\theta$ ; and (b) well location generated uniformly within plume limit.

Table 7.7 Cumulative probability distribution of receptor well depth.

Depth (m)	Cumulative Probability
4.55	0.000
4.55	0.015
6.06	0.045
6.06	0.060
9.09	0.090
9.09	0.134
10.61	0.149
10.61	0.179
12.12	0.194
12.12	0.209
15.15	0.254
20.61	0.299
21.21	0.313
21.21	0.328
22.73	0.358
22.73	0.373
24.24	0.388
24.24	0.403
27.27	0.433
27.27	0.478
30.30	0.493
30.30	0.597
39.39	0.642
39.39	0.657
45.45	0.672
45.45	0.746
60.61	0.761
60.61	0.881
71.21	0.925
75.76	0.955
75.76	0.970
90.91	1.000

For both these options, the vertical position of the observation well can be optionally constrained to lie within the approximate vertical penetration depth of the contaminant plume emanating from the waste unit. This is achieved through the Monte Carlo input variable LZCHK. If LZCHK is set to FALSE, the constraint is not enforced. If LZCHK is set to TRUE, the z-coordinate of the receptor well is constrained to lie within the approximate vertical extent of the contaminant plume as defined by

$$z_r \leq 2.5 \left\{ \frac{Q_3 + Q_4}{Q_1} B + \left[ \alpha_v (x_w + x_r) + \alpha_L \left( \frac{Q_3 + Q_4}{Q_1} B \right) + D^o \right]^{1/2} \right\} = z_{\max} \quad (7.14)$$

where

$Q_1$ - $Q_4$	=	Components of the groundwater flow field (m <sup>2</sup> /yr), see EPA (1996a), Part 2 Figure 2.3
$B$	=	Saturated zone thickness (m)
$x_w$	=	Length of source in downstream direction (m)
$x_r$	=	Horizontal distance between source and receptor well (m)
$\alpha_L$	=	Longitudinal dispersivity (m)
$\alpha_v$	=	Vertical dispersivity (m)
$D^o$	=	Molecular diffusion coefficient (m <sup>2</sup> /y)

Finally, the well position may be fixed at a constant depth. In this case a distribution code of 12 (not 0) should be entered for the vertical well position in the data input file.

## 7.14 CHEMICAL & BIOLOGICAL TRANSFORMATION COEFFICIENTS

The overall decay coefficient or the sum of the chemical and biological transformation coefficients can be expressed as a distribution or a constant value. The saturated zone derivation of the overall decay is calculated the same way as for the unsaturated zone (see Section 6.7). Although the temperature and pH values are assumed not to vary between the saturated and unsaturated zones, the porosity and bulk density values may differ, leading to a difference in the decay coefficients for the two zones. Note that the biological transformation coefficient has a default value of zero and has not been used in any EPA application to date.

## 7.15 FREUNDLICH ISOTHERM COEFFICIENT

When the adsorption isotherm is nonlinear, the user must specify two isotherm parameters: the Freundlich sorption coefficient and the Freundlich exponent (see next sub-section). A special case occurs when the isotherm is linear. In this case, the Freundlich exponent has a value of 1.0. When the isotherm is linear, the leading Freundlich coefficient is known as the solid-liquid phase distribution coefficient ( $k_d$ ). The distribution coefficient may be specified directly, or as a derived parameter. In the latter case, it is computed from the fraction organic carbon and the organic carbon partition coefficient. The following relationship is used:

$$k_d = k_{oc} f_{oc} \quad (7.15)$$

where:

$k_d$  = distribution coefficient [ $\text{cm}^3/\text{g}$ ],

$k_{oc}$  = distribution coefficient with respect to organic carbon [ $\text{cm}^3/\text{g}$ ], and

$f_{oc}$  = fraction organic carbon.

Note: The above does not apply to simulations of metals transport. In this case, the sorption isotherm is determined according to the setting of the input parameter KDEVAL. A detailed discussion of metals modeling is provided in EPA (1996c).

## 7.16 FREUNDLICH ISOTHERM EXPONENT

When a nonlinear adsorption isotherm is used, the Freundlich exponent for each chemical species must be given. No probability distribution data are currently available for this parameter. If the Freundlich exponent is omitted from the data file, it is assigned a default value of 1.0, which is equivalent to specifying a linear sorption isotherm.

## 7.17 DIFFUSION COEFFICIENT

The diffusion coefficient is set to a constant value of zero by default, but a distribution may be specified if desired.

## 7.18 ANISOTROPY

An anisotropy factor is used by the Monte Carlo module if the horizontal and vertical aquifer hydraulic conductivities are different. The relationship between horizontal and vertical conductivities is:

$$K_z = K_x/A_r$$

where:

$K_z$  = hydraulic conductivity in z direction [m/y],

$K_x$  = hydraulic conductivity in x direction [m/y], and

$A_r$  = anisotropy ratio =  $K_x/K_z$ .

The default value of  $A_r$  is 1, which indicates an isotropic system. Because anisotropy ratios observed in the field may commonly be on the order of 100:1 or even larger (Freeze and Cherry, 1979), a uniform distribution of  $A_r$  with limits of 1-100 may be reasonable. In EPACMTP, the horizontal transverse hydraulic conductivity is always set equal to the horizontal longitudinal conductivity, i.e.,  $K_y = K_x$ .

## **PART 4**

### **OUTPUT INTERPRETATION**

## 8.0 RECEPTOR WELL CONCENTRATIONS

The output of any EPACMTP run consists of predicted concentration levels, either at the water table (output from the unsaturated zone module) and/or at a receptor well(s) in the saturated zone (output from the saturated zone module). The methodology (deterministic or Monte Carlo) and application (continuous or finite source) determines the method of processing predicted concentration levels for a specific objective. The post-processing of these output results is dependent on a number of factors which are outlined and discussed in this section.

### 8.1 DETERMINISTIC MODE

In the deterministic mode, EPACMTP variables are assigned constant values and the model computes receptor well concentration which, along with the source concentration, may be used to compute a Dilution Attenuation Factor (DAF). The DAF is defined as the ratio of source concentration to receptor well concentration. For chemicals with linear adsorption, the model may be run using a source concentration value of one, so that the DAF is just the inverse of the receptor well concentration value. When a deterministic simulation is performed, the final output is single receptor concentration and generally does not require additional post processing.

### 8.2 MONTE CARLO MODE

When EPACMTP is used in the Monte Carlo mode, the primary output from the simulation model is a sequence of receptor well concentration values, where each concentration corresponds to the result of one model simulation. The Monte Carlo output is then analyzed to derive regulatory DAF values or regulatory limits on leachate and waste concentrations. Each Monte Carlo iteration yields one DAF value for the constituent of concern (plus one DAF value for each of the transformation products, if the constituent degrades to form daughter product). Since each Monte Carlo iteration has equal probability, ordering the DAF values from low to high directly yields the DAF cumulative probability distribution (CDF). If appropriate, CDF curves representing different regional distributions may be combined into a single, weighted curve that represents all regions. (See Part 3, Section 2.2 in the EPACMTP background document for further discussion, EPA 1996b.)

For a finite source scenario, the post-processing step involves determination of the paired values of leachate concentration,  $C_L$ , and total leachable waste concentration,  $C_w$ , which satisfy a specified protection level. The procedure is described in the finite source background document (EPA, 1996b). To facilitate the post-processing analysis of Monte Carlo simulations, a separate post-processing program (POSTCMTP) is distributed with the EPACMTP code and discussed in Section A.5 of Appendix A.

Several types of output files are generated when the Monte Carlo option is used. The name of the primary output file (OUTPUT.OUT) is interactively specified by the user. This file consists of two major segments:

- (1) An echo of the input data
- (2) Statistical parameters of the steady-state concentration at the receptor well (e.g., mean, median, standard deviation, selected percentiles, etc.).

This file is the one of primary interest to the user.

The second type of output file is named  $\{OUTPUT\}.CDF$  where  $\{OUTPUT\}$  is the user-specified primary output file name. This file contains a list of concentration values, sorted in ascending order, and the corresponding cumulative probability values. For steady-state, continuous source analyses this output file can be directly converted to the CDF of DAF values.

For finite source simulations the primary output required for determining leachate and waste concentration limits is contained in the  $\{OUTPUT\}n.SAT$  files. These files contain the Monte Carlo output of receptor well concentrations of each of the  $n$  different ratios of  $C_w/C_L$  that were analyzed. In other words, EPACMTP will generate  $\{OUTPUT\}1.SAT$ ,  $\{OUTPUT\}2.SAT$ , etc., corresponding to the 1st, 2nd, etc. different ratio of  $C_w/C_L$  for which EPACMTP has computed the receptor well concentration values. For a degrading contaminant, these files contain the receptor well concentrations of the parent compound, plus all daughter products.

The third type of Monte Carlo output file is named  $\{OUTPUT\}.BND$ . This optional output file contains the random variable identification code, the random variable value, and the upper and lower bounds specified for that random variable, if the random variable is generated out of bounds in either of the two subroutines RANGEN or ASSIGN. Subroutine RANGEN generates random numbers from specified probability distributions, and subroutine ASSIGN computes random variables which are derived from other random variables and constants. The  $\{OUTPUT\}.BND$  file is useful when a large number of generated and/or derived random variables occurred out of bounds, and the user wishes to see which variables these were. Note that bounds checking on the generated random variables will only be performed if the logical variables CHECK and LDRIV are set to TRUE in the Monte Carlo input file. Therefore, the  $\{OUTPUT\}.BND$  file will be empty if: (1) CHECK and LDRIV are set to FALSE, or (2) no random or derived variables are generated out of their specified bounds.

The fourth Monte Carlo output file type consists of files which contain the randomly generated values used for each Monte Carlo run. There are five of these optional files, and their names and contents are listed in Table 8.1, along with brief descriptions of the other Monte Carlo output files.

When the Monte Carlo option is used and the number of runs is greater than one, most of the EPACMTP formatted output is suppressed to limit file size and disk storage requirements to reasonable levels. However, data read from the EPACMTP input file is always echoed to the formatted output file.

### **8.2.1 Model Output Processing**

POSTCMTP is an interactive, menu-driven postprocessor for EPACMTP. It reads in the EPACMTP Monte Carlo output files, presents the results in graphical and tabular form on the screen, and provides the option to generate hard copy output on a wide variety of printers and plotters. Details on how to use EPACMTP postprocessor are presented in Section A.5.1, Appendix A.

Table 8.1 Monte Carlo output files.

Opened in	Unit No.	Name	Description
MAIN	6	User-specified	Echo of EPACMTP input, statistical parameters of receptor well concentration.
MAIN	8	{ <i>OUTPUT</i> }.CDF <sup>1)</sup>	Downgradient steady-state well concentrations sorted in ascending order and corresponding cumulative probability. (CDF of concentrations)
MAIN	13-40	{ <i>OUTPUT</i> } <i>n</i> .SAT <sup>1)</sup>	Downgradient receptor well concentrations corresponding to the <i>n</i> -th value of $C_w/C_L$ for finite source scenario.
MAIN	7	{ <i>OUTPUT</i> }.BND <sup>1)</sup>	Randomly generated or derived variables which were out of bounds.
MAIN	12	{ <i>OUTPUT</i> }.CVR <sup>1)</sup>	Values of chemical variables generated for Monte Carlo simulations.
MAIN	11	{ <i>OUTPUT</i> }.SVR <sup>1)</sup>	Values of source variables generated for Monte Carlo simulations.
MAIN	13	{ <i>OUTPUT</i> }.UVR <sup>1)</sup>	Values of unsaturated zone flow and transport variables generated for Monte Carlo simulations.
MAIN	14	{ <i>OUTPUT</i> }.AVR <sup>1)</sup>	Values of aquifer variables generated for Monte Carlo simulations.

<sup>1)</sup> {*OUTPUT*} represents the file name of the primary output file. The same file name is used, but with a different file extension to indicate the type of ancillary output file.

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## APPENDIX A

### SIMULATION USING EPACMTP: DATA INPUT GUIDE

#### A.1 GENERAL

Using EPACMTP to perform a fate and transport simulation involves the following three general steps:

1. Create input data file(s)
2. Execute EPACMTP
3. Perform post-processing output analysis

All information needed by EPACMTP to perform a simulation is read from the data input file, which is an ASCII text file. The data input file can be created using a standard ASCII text editor (Section A.2). Execution of EPACMTP is discussed in Section 7.3 and post-processing analysis is discussed in Section A.5.

#### A.2 INPUT FILE PREPARATION

Detailed format descriptions of EPACMTP data files are provided in Section A.2.1. These format instructions should be followed when using a text editor to create or change an EPACMTP data input file.

##### A.2.1 Data Input Formats

This section describes the format of data input files for EPACMTP. The data input file consists of a collection of records (a record corresponds to one line of information in the data file). There are two basic types of records. The first type of record is the data record. These records must follow in a specified order and each record must conform to a prescribed format. There are various different types of data records, each of which is distinguished by a two-character code described below. The second type of record is the comment record. Comment records are not used by EPACMTP; their purpose is to elucidate the meaning of the data records to the user and improve readability of the data file to the user. Comment records may be interspersed freely with data records.

Each record type is identified by a two-character code in the left-most 5 columns of the record. The following codes are used:

Data — Records	TI	-	Title records
	GP	-	General parameter records
	DC	-	Decay Chain data records
	OT	-	Observation Time data records
	SS	-	Source Specific data records
	FS	-	Finite Source Specific data records
	CS	-	Chemical Specific data records
	MT	-	Metals Specific data records
	US	-	Unsaturated Zone Specific data records
	AS	-	Aquifer Specific data records
**	-	Comment records	

Every record in the input file must be identified by one of the above codes. Data record groups must also be entered in the same sequential order in which they are listed above.

The formats of the data record groups are described below. In order to become familiar with the input formats, it is recommended that the user also study the example data files listed at the end of this manual.

#### **A.2.1.1 Problem Title Records**

No. of Records: As many as desired

Record Format: A5, A75

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier must be 'TI' always
6-80	TITLE	Descriptive title for problem

#### **A.2.1.2 General Parameter Records**

Record No. GP01: Control Parameters

Format: A5, L5, 5I5, 2L5, I5

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be 'GP' always
6-10	MC	Monte Carlo control parameter = F(false) for deterministic run = T(true) for Monte Carlo run (Default).

11-15	IVADOS	Control parameter for unsaturated zone simulation. = 0 if <u>no</u> unsaturated zone modeling is required, = 1 if unsaturated zone modeling is required (Default).
16-20	ISTMOD	Control parameter for saturated zone simulation. = 0 if <u>no</u> saturated zone modeling is required, = 1 if saturated zone modeling is required (Default).
21-25	NSPECI	Number of contaminant component species in the system. Default = 1.
26-30	KFDM	Simulation method = 0, finite element = 1, finite difference
31-35	KFS	Control parameter for selecting continuous (infinite) source or finite source modeling option = 0 for continuous source option = 2 for landfill finite source option.
36-40	FULL3D	Logical control parameter for selecting fully 3D or quasi-3D saturate zone modeling option = T(rue) for fully 3D simulation = F(alse) for quasi-3D simulation Note: FULL3D = F(alse) should be used for Monte Carlo simulations
41-45	METAL	Logical control parameter for metals simulation = T(rue) for metals modeling = F(alse) for non-metals modeling
46-50	KDEVAL	Integer control parameter for selecting the scheme for determining the metals sorption isotherm (Leave blank if METAL = FALSE) = 1 Use the method of Loux for calculating $k_d$ from pH = 2 Use linearized MINTEQA2 isotherm = 3 Use nonlinear MINTEQA2 isotherm

51-55	LTCHK	Logical variable to check minimum transmissivity = F (alse) if no = T (rue) if yes (default)
56-60	IFREGNL	Logical variable for Regional Site-based Analysis = F (alse) for Nationwide Analysis = T (rue) if yes (default)
61-65	ISRC_TYP	Control parameter for selecting the type of waste source = 0 for landfill = 1 for surface impoundment = 2 for waste pile = 3 for land treatment

Notes:

- 1) MC is a logical variable: it should be set to either 'F' or 'T' (right-justified in input field).
- 2) The maximum number of component species that the code can handle is seven (NSPECI=7).
- 3) The default option FULL3D=FALSE reduces CPU time and memory requirements of the EPACMTP code.
- 4) Finite source option A (KFS=0) selects the methodology developed for EPACML (see EPA, 1993).  
  
Finite source option B (KFS=1) selects the methodology developed for EPACMTP (see EPA, 1992: Background document for EPACMTP: Finite Source Methodology for degrading chemicals with transformation products).
- 5) The different options for metals modeling are documented and explained in the metals background document for EPACMTP (EPA, 1996d).
- 6) If IFREGNL = True option is selected, regional site-based parameters must be supplied in a Input data file. The records in the data file are arranged under the following codes:
  - DP contains information on number of sites, climatic and groundwater regions.
  - SP Contains site areas, depths, groundwater temperature and their corresponding site-climatic regions, groundwater regions and weights
  - IN Infiltration rates for different soil types for different climatic regions
  - RE Recharge rates for different soil types for different climatic region
  - HG Groundwater hydrological parameters, hydraulic gradient, unsaturated and saturated zone thickness and aquifer hydraulic conductivity

Sample data file listing is provided in Appendix A.

Record No. GP02: Monte Carlo Control Parameters

\*\*\* Omit this record for a deterministic \*\*\*  
model run (MC = F(false))

Format: A5, I5, 7L5, F10.0

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be 'GP' always
6-10	NRUN	Number of iterations in Monte Carlo run. Recommended value is 1000 or greater.
11-15	ECHO	Logical variable for creating output 'VR' files. = F(false) if no; VR files should not be created (Default), = T(true) if yes; VR files should be created.
16-20	CHECK	Logical variable indicating if generated random variables are restricted to lie within specified upper and lower bounds, = F(false) if no, = T(true) if yes (Default).
21-25	CORR	Logical variable indicating if statistical correlation is to be used in generating unsaturated zone parameters, = F(false) if no (Default), = T(true) if yes.
26-30	LDRIV	Logical variable indicating if derived Monte Carlo variables are constrained to lie within specified upper and lower bounds, = F(false) if no (Default), = T(true) if yes.
31-35	LYCHK	Logical variable indicating if observation well is constrained to lie within the approximate areal extent of the plume, = F(false) if no, = T(true) if yes (Default).

36-40	LZCHK	<p>Logical variable indicating if observation well depth is constrained to lie within the approximate vertical plume depth.</p> <p>= F(false) if no (Default), = T(true) if yes.</p>
41-45	LBNDOT	<p>Logical variable indicating if the '.BND' output file is to be created,</p> <p>= F(false) if no (Default), = T(true) if yes.</p>
46-50	ALLRUN	<p>Logical control parameter to set aggregation option</p> <p>= T(true) to automatically aggregate Monte Carlo results over all soil and cover types = F(false) to perform run only for the selected soil and cover type.</p>
51-60	TCUTOFF	<p>Value of the upper time limit, in years, for determining the receptor well maximum concentration in finite source modeling.</p>

Notes:

- 1) If the ALLRUN = True option is selected, silt-loam infiltration rate and recharge rate values in the source-specific group must be used. The soil parameters in the unsaturated zone specific group must also be set to the values for the silt loam soil type. ALLRUN is not used if the regional site-based analysis is selected (IFREGNL=True).
- 2) The option to incorporate statistical correlation while generating unsaturated zone parameters (CORR = (T)true) has not been implemented in this version of EPACMTP; hence, always set CORR = (F)false.

Record No. GP03: Deterministic Control Parameters

\*\*\* Omit this record if a Monte Carlo simulation \*\*\*  
is performed with continuous source condition  
(MC=T(rue) and KFS=0)

Format: A5, 7I5, G10.0, 2I5

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be 'GP' always.
6-10	ISBC	Contaminant source boundary condition = 0 if contaminant flux is given (Default), = 1 if contaminant concentration is given.
11-15	IBAT	Control parameter for decaying source boundary condition, = 0 if no (continuous source or non-degrader infinite source) = 1 Biochemical decay (hydrolysis) = 2 Physical decay due to leaching (source depletion) = 3 Combine 1+2 (IBAT >=1 for degrader finite sources) Note: If IBAT = 1 or 3 is selected, it is assumed that the effective hydrolysis transformation coefficients in the waste source are the same as in the unsaturated and saturated zone.
16-20	IUSTED	Control parameter indicating whether transport in the unsaturated zone is steady-state or transient, = 0 for transient (if KFS=1 or 2), = 1 for steady-state (if KFS=0). Leave blank if IVADOS (see record GP01)=0.
21-25	ISSTED	Control parameter indicating whether transport in the saturated zone is steady-state or transient = 0 for transient (if KFS=1 or 2) = 1 for steady-state (if KFS=0). Leave blank if ISTMOD (see record GP01) = 0.
26-30	NUTOBS	Number of time values at which concentration at the water table is to be computed Leave blank if ISTMOD = 1, and/or IUSTED=1, and/or MC=T(rue).
31-35	NTS	Number of time values at which receptor well concentrations in the saturated zone are to be computed Leave blank if ISTMOD=0, or ISSTED=1.

Note: Set NTS = -1 or 0 to run finite source option in Monte-Carlo mode.

36-40	NWELLS	Number of receptor wells in the saturated zone. Leave blank if ISTMOD (see record GP01) = 0.
41-45	QRMAX	Maximum groundwater vertical flux ratio (see Eq. 2.3.34) for selecting between analytical and numerical saturated zone contaminant transport solution. Recommended value is 0.02. Leave blank if ISTMOD (see record GP01) = 0.
51-55	NRATIO	Number of ratios of $C_w/C_L$ to be used for finite source scenario (KFS=2). Default value is 8. Leave blank for a continuous source analysis (KFS=0) or a finite source analysis with a constant source leaching duration.
56-60	ICRW	Control parameter indicating the time-dependent receptor well concentration to be computed for the finite source analysis = 0 compute peak receptor well concentration (Default) = 1 compute temporally averaged receptor well concentration When ICRW=1 is used, the averaging period for each of the species must be specified in variable CARC, in the chemical-specific data records. The default period is 70 years.

Notes:

- 1) The maximum value for NUTOBS is 20. NUTOBS is automatically set to 0 if a steady-state simulation is performed (IUSTED=1).
- 2) The maximum value for NTS is 60. NTS is automatically set to 1 if a steady-state simulation is performed (ISSTED=1).
- 3) The maximum value for NWELLS is 40.
- 4) The maximum value for NRATIO is 9.

**A.2.1.3 Finite Source Data Records**

When the finite source option is selected, with KFS=2 (see record FP01), the following additional data record group is required. The finite group is indicated by the record identifier "FS". The record group contains the values of the ratios  $C_w/C_L$  that are to be used in the analysis.

Format: A5,8G10.0

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be "FS" always.

6-15,	CRATIO(1)	Sequential values (in increasing order) of the ratios $C_w/C_L$ to be used in the finite source Monte Carlo analysis.
16-25	.	
.	.	
etc.	CRATIO (NRATIO)	

Note: Up to 8 values can be entered on one line; if the value of NRATIO is greater than 8, the data record should be repeated, but without the group code.

#### A.2.1.4 Chain Decay Data Records (DC)

\*\*\*\*\*

This entire group is used only for chain decay modeling with multiple contaminant species (NSPECI > 1). Omit this group if NSPECI = 1.

\*\*\*\*\*

The following input records, DC01 through DC03, are to be repeated a total of NSPECI-1 times, for each of the component species in the decay chain, except the first component species.

Record No. DC01: Number of Parent Species

Format: A5, 2I5

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be 'DC' always.
6-10	I	Species number, from 2 to NSPECI.
11-15	NPA(I)	Number of immediate parents for I-th species.

Record No. DC02: Parent Numbers

\*\*\* Omit this record if the number of parents (NPA) = 0 for the current species \*\*\*

Format: 4I5

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be 'DC' always.

6-10	KPAREN(I,1)	Sequential species numbers of the immediate parents of the current species, where NUMPAR = NPA(I).
.	.	
.	.	
.	.	
21-25	KPAREN(I,NUMPAR)	

Record No. DC03: Decay Speciation Factors

\*\*\* Omit this record if the number of parents (NPA) = 0 for the current species \*\*\*

Format: A5, 4G10.0

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be 'DC' always.
6-15	APAREN(I,1)	Fraction of each parent that decays into species I, where NUMPAR = NPA(I).
.	.	
.	.	
36-45	APAREN(I,NUMPAR)	

#### **A.2.1.5 Observation Time Records (OT)**

\*\*\*\*\*

Omit this group when a Monte Carlo simulation is performed (MC = TRUE).

\*\*\*\*\*

Record No. OT01: Unsaturated Zone Concentration Output Times

\*\*\* Omit this record when unsaturated zone simulation is not performed (IVADOS = 0. see record GP01).

Format A5, 8G10.0

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be 'OT' always
6-15, 16-25	UTOBS(1)	Time values for which concentrations are to be computed.
.	.	
.	.	
etc.	UTOBS(NUTOBS)	

Note: The maximum allowed value for NUTOBS is 20. Up to eight time values can be entered on each line of the input file. This record should be repeated as many times as necessary (maximum of 3) to enter all time values.

Record No. OT02: Saturated Zone Observation Time Values

\*\*\* Omit this record if only unsaturated zone \*\*\*  
simulation is performed (ISTMOD = 0, see  
record GP02)

Format: A5, 8G10.0

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Record identifier; must be 'OT' always
6-15 11-20, etc.	T(1) . . T(NTS)	Time values for which concentrations in saturated zone observation wells are to be computed.

Note: The maximum allowed value for NTS is 60. Up to eight time values can be entered on each line of the input data file. This record should be repeated as many times as necessary (maximum of 8) to enter all time values.

**A.2.1.6 Source-Specific Data Records (SS)**

The records in this group contain the parameters that describe the contaminant source. Records in this group are identified by the code 'SS'. All records in this group have a common format which is described in Table A.6. Each record in the group corresponds to one source parameter. To indicate this correspondence, each source parameter is assigned a number. The appropriate number is entered as the second variable (IVAR) of each record following the record identifier.

A list of the records (parameters) in the source specific data group is given below in Table A.1.

Table A.1 Input parameters for source-specific group. See Table 7.6 for data input formats.

IVAR	EPACMTP Parameter	Description
1	AREA	Area of disposal unit (m <sup>2</sup> )
2	XW	Length (x-direction) of disposal unit (m)
3	YD	Width (y-direction) of disposal unit (m)
4	CZERO(I)	Leachate concentration emanating from the waste disposal facility (mg/L). For a degrading constituent, this record should be repeated for the parent and all daughter products, i.e., NSPECI times. For finite source degrader simulations CZERO represents the initial leaching concentration; the value should be set to zero for all daughters. The value for the parent should be set to a large value (10 <sup>6</sup> is presently used) to avoid numerical difficulties associated with very small concentration values for degrading constituents. The value specified in the data input file is a dummy value only; the Monte Carlo results are adjusted for a range of actual C <sub>L</sub> values as a post-processing step.
5	RECHRG	Areal recharge rate (m/y)
6	SINFIL	Infiltration rate from disposal unit (m/y)
7	HZERO	Ponding depth of surface impoundment unit (m)
8	DLINR	Thickness of liner (m)
9	CLINR	Hydraulic conductivity of liner (m/y)
10	TSOURC	Duration of leaching period (y) for finite source option (KFS=1)TSOURC should be specified as a <u>derived</u> variable if KFS=2 (i.e. for landfills).

Table A.1 Input parameters for source-specific group. (continued)

IVAR	EPACMTP Parameter	Description
11	DEPTH	Depth of the waste disposal facility (m) for landfill finite source option.
12	FRACT	Fraction of hazardous waste in the waste disposal facility for landfill finite source option.
13	PWS	Dummy parameter.
14	CTDENS	Density of hazardous waste (g/cm <sup>3</sup> )

Notes:

- 1) For a deterministic simulation with decaying source conditions (IBAT = 1, see group GP04), CZERO represents the initial concentration.
- 2) Parameters 7-9 (HZERO, DLINR, CLINR) are required only for the surface impoundment scenario when an unsaturated zone simulation is performed (IVADOS=1, see group GP01) and the source ponding option is used. In this case, parameter 6 (SINFIL) should be specified as a derived parameter.

### A.2.1.7 Chemical-Specific Data Records (CS)

The records in this group contain the parameters that describe the degradation, adsorption and diffusion characteristics of each of the chemical species being simulated. Records in this group are identified by the code 'CS'. All records in this group have a common format which is described in Table A.6. Each record corresponds to one chemical specific parameter. To indicate this correspondence, each chemical specific parameter is assigned a number. The appropriate number is entered as the second variable (IVAR) of each record. A list of records (parameters) in the chemical specific group is provided below in Table A.2.

Table A.2 Input parameters for chemical-specific group. See Table A.6 for data input formats.

IVAR	EPACMTP Parameter	Description
1	RLAM2(I)	Sorbed phase hydrolysis decay rate (1/y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
2	RLAM1(I)	Dissolved phase hydrolysis decay rate (1/y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
3	AHYDR(I)	Second-order acid catalyzed hydrolysis rate constant at reference temperature (1/mol-y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
4	NHYDR(I)	Neutral hydrolysis rate constant at reference temperature (1/y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
5	BHYDR(I)	Second-order base catalyzed hydrolysis rate constant at reference temperature (1/mole-y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
6	RTEMP	Reference temperature (°C).
7	KOC(I)	Normalized distribution coefficient for organic carbon (ml/g). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.

Table A.2 Input parameters for chemical-specific group. (continued)

IVAR	EPACMTP Parameter	Description
8	DSTAR(I)	Effective molecular diffusion coefficient ( $m^2/y$ ). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
9	DWS(I)	Drinking water standard (mg/L), i.e., HBL or MCL value for comparison against model predicted average receptor well concentrations. For a degrader, this record should be repeated for the parent and all daughter products, i.e., NSPECI times.
10	CARC(I)	Base exposure period (y) for calculating average receptor well concentration. Set to 70 y for carcinogens, and 35 y for non-carcinogens. Always specify this parameter as a constant. For a degrader, this record should be repeated for the parent and all daughter products, i.e., NSPECI times.

Notes:

- 1) The parameters 1-7 in this group are used to compute degradation rates and partition coefficients for each of the contaminant component species. These parameters are required only when the overall degradation rate and sorption parameters for the unsaturated and saturated zone, (see groups US and AS) are given as derived parameters, otherwise this group may be omitted.
- 2) If variables 1-2 (RLAM2 and RLAM1) are specified as derived parameters, they will be computed from the acid, neutral and base catalyzed hydrolysis rates (variables 3-5).
- 3) If variables 1-2 (RLAM2 and RLAM1) are specified as random with statistical distributions, variables 3-6 (hydrolysis rates) are not used, and may be omitted.
- 4) If the adsorption isotherm is linear, the partition coefficient can be calculated from the  $K_{oc}$  value (variable 7). If on the other hand, the isotherm is nonlinear, the Freundlich isotherm parameters for the unsaturated and saturated zone must be given themselves in the record groups 'US' and 'AS', respectively. In this case the  $K_{oc}$  is not used and may be omitted.
- 5) For a multispecies simulation, it is required that the degradation and sorption parameters for all species are specified in a consistent manner. For instance, if the degradation rate for the first species is a derived parameter and computed from the acid, neutral and base catalyzed hydrolysis rates (variables 3-5), this same procedure must also be used for the remaining species.

- 6) Chemical-specific variable CARC (IVAR = 10) is not required when a steady-state (infinite source) analysis is performed, or when the finite source analysis uses the peak instead of time-averaged receptor well concentration (ICRW=0, see input group GP03).

#### A.2.1.8 Metals-Specific Data Record (MT)

The records in this group contain the parameters that describe the master variables that control the selection of the effective metals sorption isotherm. Records in this group are identified by the code 'MT'. All records in this group follow the format described in Table A.6. Each record corresponds to one parameter. To indicate this correspondence, each metal specific parameter is assigned a number. The appropriate number is entered as the second variable (IVAR) of each record, following the record identifier. A list of records (parameters) in the metals-specific group is given below in Table A.3.

Table A.3 Input parameters for metals specific group. See Table A.6 for data input formats.

IVAR	EPACMTP Parameter	Description
1	METAL_ID	Identification number for the metal.
2	USPH	Soil and aquifer pH.
3	FEOX	Weight percentage of iron-hydroxide in the soil and aquifer.
4	LOM	Concentration (mg/L) of dissolved organic carbon in the waste leachate.
5	USNOM	Unsaturated zone percentage organic matter.
6	ASNOM	Aquifer fraction organic carbon.

#### Notes:

- 1) This group is required only for metals modeling (METALS = True, see group GP01); the group may be omitted if METAL = F(alse).
- 2) Presently the following METAL\_ID codes are recognized: 1 = Barium; 2 = Cadmium; 3 = Chromium (4+); 4 = Mercury; 5 = Nickel; 6 = Lead; 7 = Silver; 8 = Zinc (6+); 9 = Copper; 10 = Vanadium; 13 = Arsenic; 14 = Chromium (tb); 15 = Selenium; 16 = Thallium; 17 = Antimony.
- 3) The unsaturated zone percentage organic matter varies with soil type and should be the same as that specified under the unsaturated zone specific group (see section 6.4.5).
- 4) The saturated zone fraction organic carbon should be the same as that specified under the aquifer specific group (see section 7.5.12).

### A.2.1.9 Unsaturated Zone Specific Data Record (US)

The records in this group contain the parameters that describe unsaturated zone physical and chemical characteristics. Records in this group are identified by the code 'US'. All records in this group follow the format described in Table A.6. Each record corresponds to one unsaturated zone parameter. To indicate this correspondence, each unsaturated zone parameter is assigned a number. The appropriate number is entered as the second variable (IVAR) of each record, following the record identifier. A list of records (parameters) in the unsaturated zone specific group is given below in Table A.4.

Table A.4 Input parameters for unsaturated zone specific group. See Table A.6 for data input formats.

IVAR	EPACMTP Parameter	Description
1	SATK	Saturated hydraulic conductivity, $K_s$ , (cm/hr).
2	ALPHA	Moisture retention parameter, $\alpha$ , ( $\text{cm}^{-1}$ ).
3	BETA	Moisture retention parameter, $\beta$ .
4	WCR	Residual water content, $\theta_r$ .
5	WCS	Saturated water content, $\theta_s$ .
6	DSOIL	Thickness of unsaturated zone (m).
7	DISPR	Dispersivity, $\alpha$ , (m)
8	POM	Percent organic matter
9	RHOB	Bulk density, $\rho_b$ , ( $\text{g}/\text{cm}^3$ )
10	UFCOF(I)	Leading coefficient in Freundlich adsorption isotherm, $k_1$ . For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
11	UFEXP(I)	Freundlich exponent, $\eta$ . For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
12	UCLAM(I)	Chemical degradation rate coefficient (1/y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.

Table A.4 Input parameters for unsaturated zone specific group. (cont)

IVAR	EPACMTP Parameter	Description
13	BIOU(I)	Biological degradation rate coefficient (1/y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.

Notes:

- 1) This group may be omitted if no unsaturated zone simulation is performed (IVADOS=0, see group GP02).
- 2) If the adsorption isotherm is linear, variable 11(UFEXP) should be omitted or set to a constant value of 1.0. In this case, variable 10 (UFCOF) corresponds to the partition coefficient,  $k_d$ , ( $\text{cm}^3/\text{g}$ ).
- 3) IF UFCOF is specified directly (i.e., not derived), variable 8 (POM) may be omitted.
- 4) If the chemical degradation rate (UCLAM) is specified as a derived parameter, it will be calculated from the chemical specific decay parameters (CS-group).
- 5) For a multispecies simulation, it is required that the degradation and adsorption parameters for all species are specified in a consistent manner. For instance, if the chemical degradation rate for the first species is specified directly instead of derived, the same procedure must be used for the remaining species.

#### A.2.1.10 Aquifer-Specific Data Records (AS)

The records in this group contain the parameters that describe the saturated zone physical and chemical characteristics. Records in this group are identified by the code 'AS'. All records in this group follow the format described in Table A.6. Each record corresponds to one saturated zone parameter. To indicate this correspondence, each saturated zone parameter is assigned a number. The appropriate number is entered as the second variable (IVAR) of each record, following the record identifier. A list of records (parameters) in the saturated zone specific group is given below in Table A.5.

Table A.5 Input parameters for aquifer specific group. See Table A.6 for data input formats.

IVAR	EPACMTP Parameter	Description
1	DIAM	Average particle diameter (cm)
2	POR	Aquifer porosity
3	BULKD	Aquifer bulk density (g/cm <sup>3</sup> )
4	ZB	Aquifer Saturated thickness (m)
5	XKX	Longitudinal hydraulic conductivity, $K_x$ , (m/y)
6	ANIST	Anisotropy ratio, $K_x/K_z$
7	GRADNT	Hydraulic gradient (m/m)
8	VXCS	Regional groundwater <u>seepage</u> velocity (m/yr)
9	RETARD(I)	Retardation coefficient. For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times
10	AL	Longitudinal dispersivity, $\alpha_L$ (m)
11	AT	Transverse dispersivity, $\alpha_T$ (m)
12	AV	Vertical dispersivity, $\alpha_v$ (m)
13	TEMP	Temperature of ambient aquifer water (°C)
14	PH	Ambient groundwater pH
15	FOC	Fraction organic carbon (g/g)
16	RADIS(I)	Radial distance of observation well from center of downstream edge of waste disposal unit (m). Repeat this record for each of the NWELLS observation wells.
17	ANGLE(I)	Angle off-center of observation well measured counterclockwise (degrees). Repeat this record for each of the NWELLS observation wells.
18	XWELL(I)	Distance in downstream direction (m) between downstream edge of the source and observation well. Repeat this record for each of the NWELLS observation wells.

Table A.5 Input parameters for aquifer specific group. (continued)

IVAR	EPACMTP Parameter	Description
19	YWELL(I)	Horizontal transverse distance of well from the plume centerline (m). Repeat this record for each of the NWELLS observation wells.
20	ZWELL(I)	Depth of well below water table (m). Repeat this record for each of the NWELLS observation wells. Note ZWELL should be given as a fraction of the saturated zone thickness, unless distribution type 12 (Section 6.5.13), i.e. constant well depth, is being used.
21	SFCOF(I)	Leading coefficient of Freundlich adsorption isotherm (distribution coefficient). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
22	SFEXP(I)	Freundlich isotherm exponent. For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
23	CSLAM(I)	Chemical degradation rate coefficient (1/y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.
24	BIOS(I)	Biodegradation rate coefficient (1/y). For a multispecies simulation, this record should be repeated for each of the components in the decay chain, i.e., NSPECI times.

Notes:

- 1) This entire group may be omitted when no saturated zone simulation is performed (ISTMOD=0, see group GP01).
- 2) For a Monte Carlo simulation, only one observation well is allowed.
- 3) The x-(longitudinal or downstream) and y-(horizontal transverse) location of the observation well(s) relative to the source can be determined in two ways. The first way is to give the x- and y-locations directly, through variables 18 and 19. The second way is to give these locations in terms of the radial distance between the well(s) and the center of the downstream side of the

source, and the angle between this radial direction and the x-direction (see figure 6.1). If the latter option is used, the x and y locations (variables 18 and 19) should be given as derived variables.

- 4) If the adsorption isotherm is linear, the Freundlich coefficient, SFEXP(I), should be set equal to 1.0 or omitted. In this case, SFCOF(I) corresponds to the partition coefficient  $k_d$ .
- 5) If the retardation coefficient (RETARD) is specified directly and not a derived parameter, then SFEXP, SFCOF and FOC can be omitted. This is valid only when the isotherm is linear.
- 6) When the degradation rate is not a derived parameter, the aquifer pH is not needed.
- 7) For a multispecies simulation, it is required that the degradation and adsorption parameters for all species are specified in a consistent manner. For instance, if the chemical degradation rate for the first species is specified directly instead of derived, the same procedure must be used for the remaining species. It is allowed that the sorption isotherm for some species is linear, while it is nonlinear for other species. In this case the isotherm parameters SFCOF and SFEXP must be specified for all species.

### A.3 EMPIRICAL DISTRIBUTIONS DATA RECORDS (EM)

\*\*\*\*\*

Omit this group for a deterministic simulation (MC=False) or if no empirical distributions were specified in input groups SS-AS.

\*\*\*\*\*

#### (i) Header record

No. of records: 1                      Format: 2A5, 2I5

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Data input group identifier. Should be 'EM' always.
6-10	EMPCOD	Character variable indicating to which parameter group the empirical distribution belongs; enter SS, CS, US or AS.
11-15	IEMP	Integer variable indicating parameter number (IVAR) to which the empirical distribution corresponds.
16-20	NPT	Number of entry pairs of random values and cumulative probabilities for empirical distribution.

#### (ii) Data records

No. of records: NPT                      Format: A5, 2G10.0

<u>Col.</u>	<u>Variable</u>	
1-5	GRPCOD	Data input group identifier. Should be 'EM' always.
6-15	VALUE (J,I)	Value of J-th point in empirical distribution.
16-25	CDF (J,I)	Cumulative probability of J-th point.

Notes:

- 1) Both the header and data records are to be repeated for each of the specified empirical distributions in groups SS through AS.
- 2) The empirical distributions must be entered in the same consecutive order in which they appear in groups SS through AS.

Table A.6 Data format for input records in groups SS, CS, US and AS.

---

Format: A5, 2I5, 4G10.0, A25

---

Col.	1-5	GRPCOD:	Character variable code to indicate group type of random variable; enter SS, CS, US, or AS.
	6-10	IVAR:	Integer variable indicating which EPACMTP input parameter the record corresponds to.
	11-15	IDIST:	Integer variable indicating type of statistical distribution (see Table 5.1).
	16-25	MEAN:	Specified mean of statistical distribution.
	26-35	SD:	Standard deviation of statistical distribution.
	36-45	LOWER:	Lower bound of statistical distribution.
	46-55	UPPER:	Upper bound of statistical distribution.
	56-80	VARNAM:	Character variable giving name of the EPACMTP parameter to which record corresponds.

---

Notes:

- 1) The first variable of each record is a two-character string that identifies the input group, e.g. 'CS'.

- 2) The second variable gives the parameter number. Each EPACMTP parameter has a number that is unique within each group. This number is used by the code to identify the correct model parameter.
- 3) The third variable determines whether the parameter should be held constant ( $IDIST=0$ ), or be considered a Monte Carlo variable ( $IDIST \geq 1$ ). A negative value indicates that the parameter is derived, i.e., computed from another EPACMTP input parameter. The codes used are described in Table 5.1. This variable is ignored during a deterministic simulation, unless the parameter is derived (indicated by a negative distribution code).
- 4) The fourth variable gives the mean of the probability distribution for a Monte Carlo simulation, and the actual parameter value to be used for a deterministic simulation, or when the parameter is held constant. This variable is not used when the parameter is derived.
- 5) The fifth variable gives the standard deviation of the probability distribution for a Monte Carlo simulation. This variable is not used when the parameter is held constant or for a deterministic simulation.
- 6) The sixth and seventh variable correspond to the lower and upper bounds, respectively, of the probability distribution of the parameter. Setting both to zero means that the bounds will be ignored by EPACMTP. They are not used for a deterministic simulation or when the parameter is held constant.
- 7) The eighth and final variable for each record is an optional 25-character string that may be used to identify the model parameter corresponding to the input record.
- 8) The input records and parameters for each of the source specific (SS), Chemical Specific (CS), Unsaturated zone Specific (US), and Aquifer Specific (AS) input groups are listed in Tables A.1 through A.5.

It is useful to note that often, especially while performing deterministic simulations, the model may not require input records for each and every parameter described above. For instance, the source area can be omitted if the x- and y-dimensions of the source are given individually. If an input parameter is not actually used by EPACMTP, and its corresponding record is still present in the data file, EPACMTP will simply skip this record. To determine whether an input record is required or not, the user must be aware of the possible dependencies between input parameters. This is especially important for derived parameters. Failure to enter all necessary records/parameters may lead to unpredictable results!

#### **A.4 RUNNING EPACMTP**

EPACMTP can be used to simulate either a single problem at a time, or to process a number of problems in batch mode. When EPACMTP is started, the code will first ask the user whether a batch run is desired. If the user returns N(o), a single problem (either Monte Carlo or deterministic) will be simulated. The user is then prompted by EPACMTP to provide the name of the input data file containing the problem definition, and the name to be given to the output file.

If a batch run is selected, the user must provide the name of the batch file. The batch file is simply a separate file containing a list of all the EPACMTP data input files that are to be processed in the batch run. EPACMTP will then sequentially execute all the input data files in the batch file. The output files for each problem will be created automatically; they will have the same file name as the data input file, but with different extensions.

## **A.5 MODEL OUTPUT POST PROCESSING**

The output from EPACMTP consists of predicted concentration levels, either at the water table (output from the unsaturated zone module), and/or at observation wells located in the saturated zone (output from the saturated zone module). When a deterministic simulation is performed, all output is written to the primary output file, and generally does not require additional post processing. When a Monte Carlo simulation is performed, the output of interest consists of the receptor well concentration values generated by each individual simulation. For continuous source runs, the entire cumulative distribution function (CDF) of the receptor well concentrations is written to the *{OUTPUT}.CDF* file.

For finite source runs, the Monte Carlo output is written to a series of *{OUTPUT}n.SAT* files, with each file corresponding to a different value of the ratio between total waste and leachate concentration. These files are subsequently used by POSTCMTP post-processor to provide the regulatory limits on waste and leachate concentration for any protection level. It may be noted that the finite source option of POSTCMTP does not allow aggregation of Monte Carlo results. Rather, it is assumed that the aggregation has already been performed inside EPACMTP, using the ALLRUN option of the model. ALLRUN option is set to FALSE when regional site-based analysis is performed, i.e. IFREGNL=TRUE.

### **A.5.1 Using POSTCMTP**

POSTCMTP is an interactive, menu-driven postprocessor for EPACMTP. It reads in the EPACMTP Monte Carlo output files and presents the results in graphical and tabular form on the screen, and also provides the option to generate hard copy output on a wide variety of printers and plotters.

To use the postprocessor, simply type 'POSTCMTP'. The first time you run the program, you will automatically be taken into the setup menu to select the type of printer you have and to specify how it is connected to your PC. After completing the initial setup, you can always change the configuration by selecting the '(I)nitialize Plotting Device' option from the main menu. The main menu also allows you to select either '(C)ontinuous Source Analysis' or '(F)inite Source Analysis'. You must select the analysis type that corresponds to the EPACMTP Monte Carlo simulation that you want to analyze. For example, it is not valid to select (F)inite Source Analysis if a steady-state Monte Carlo run was performed.

## Continuous Source Analysis

After selecting the (C)ontinuous Source option, you will be prompted to provide the name of the EPACMTP output file. You must enter the file name only, without an extension. After entering the filename, select the (G)raph option to view the simulated DAF curve. After the graph has been drawn on the screen, you can either save the graph on disk using the (S)ave option, or send the graph to your printer or plotter using the (H)ard Copy option. Please note that printing on a laser printer is quite slow; it may take more than 5 minutes to complete the plot.

From the (C)ontinuous Source menu, you may also press the (S)pecify option. This allows you to compute the DAF at any arbitrary level of probability, or to compute the probability that the DAF will exceed a specified value.

Press (E)xit to return to the POSTCMTP main menu.

## Finite Source Analysis

After selecting the (F)inite Source Analysis option from the main menu, you will first be asked to supply the name of the EPACMTP output file you want to analyze. This file name must be entered without the file extension. After reading in the files, the program will perform the finite source post-processing analysis. By default, it will compute the values of total waste concentration ( $C_w$ ) and leachate concentration ( $C_l$ ) that correspond to an 85th percentile protection level. To change this, select the (S)pecify option, and enter the desired protection level.

To view the post-processing results graphically, select the (G)raph option. After the graph has been drawn on the screen, you may (S)ave the graph on disk, or print it on you printer or plotter using the (H)ard Copy option. Please note that printing to a laser printer is quite slow; it may take more than 5 minutes to complete the plot.

Press (E)xit to return to the Main POSTCMTP menu.

## **APPENDIX B**

### **INPUT AND OUTPUT FILES FOR A MONTE CARLO ANALYSIS SAMPLE PROBLEM**

## APPENDIX C

### FREQUENCY DISTRIBUTIONS OF MONTE CARLO INPUT PARAMETERS

This Appendix contains frequency distribution plots of EPACMTP input parameters. The plots are represented in the form of histograms that display different intervals of parameter values and the corresponding frequency of observation. The observation frequency is given as a fraction of the total population. For example, a normalized frequency of 0.50 means that the corresponding interval contains half of the total population. The length of each interval is the distance between the mid points of two successive bars.

A log scale axis has been used in some plots in order to achieve appropriate representation of the range of values for some of the input parameters such as area, hydraulic conductivity, and hydraulic gradient.

The data used to plot the frequency distributions of the source related parameters (area, depth, infiltration, and recharge) is unique for each waste management scenario (landfills, surface impoundments, and land application units). Data for the area and depth were obtained from the OPPI Survey database. Infiltration and recharge rates were computed by the HELP model for individual waste management scenarios. The data for unsaturated and saturated zone parameters is the same for all waste management scenarios and represent nationwide distributions, obtained through aggregation of the distributions of the twelve individual hydrogeological environments. The values were generated by running EPACMTP in Monte Carlo mode.