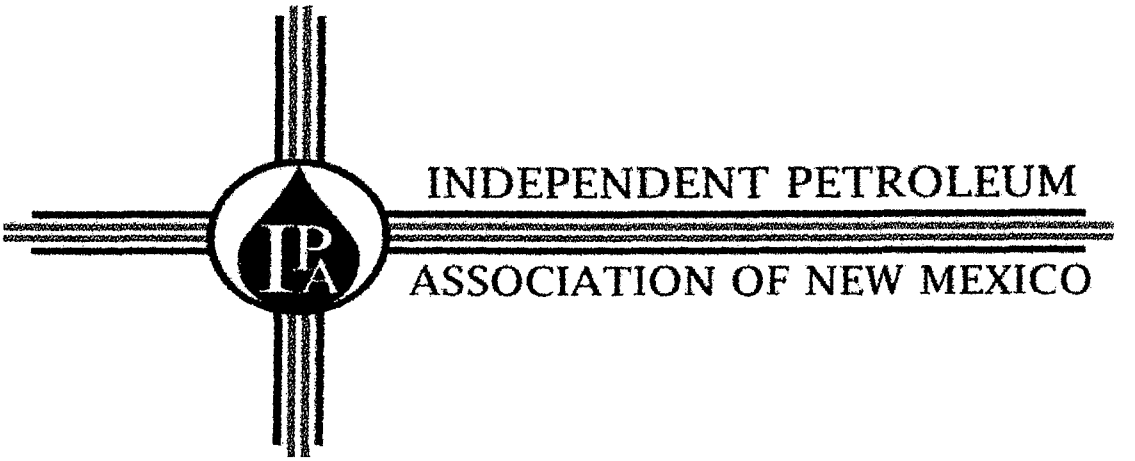


OCD CASE NOS. 14784 AND 14785

IPANM Petition to amend Title 19, Chapter 15, part 17 (The PIT Rule)

May 14 – 18, 2012

IPANM exhibit 9
MULTIMED Model Manual
- Two Hundred Twenty Two (222) pages -

EPA
August 1990

A SUBTITLE D LANDFILL APPLICATION MANUAL FOR THE MULTIMEDIA EXPOSURE ASSESSMENT MODEL (MULTIMED)

by

Susan Sharp-Hansen[1]
Constance Travers[1]
Paul Hummel[1]
Terry Allison[2]

AQUA TERRA Consultants[1]
Mountain View, CA 94043

Computer Sciences Corporation[2]
Athens, GA 30605-2720

EPA Contract No. 68-03-3513

Project Monitor

Gerard Laniak
Environmental Research Laboratory
U.S. Environmental Protection Agency
Athens, GA 30605-2720

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GEORGIA 30605-2720

DISCLAIMER

The work presented in this document has been funded by the United States Environmental Protection Agency. It has been subject to the Agency's peer and administrative review, and has been approved as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use by the U.S. Environmental Protection Agency.

FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient management tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact and control of environmental contaminants, the Assessment Branch develops management or engineering tools to help pollution control officials assess the risk to human health and the environment posed by land disposal of hazardous wastes.

EPA's Multimedia Exposure Assessment (MULTIMED) simulates the transport and transformation of contaminants released from a hazardous waste disposal facility into the multimedia environment. MULTIMED includes contaminant release to either air or soil and possible interception of the subsurface plume by a surface stream. An important application of MULTIMED would be the prediction of pollutant movement in leachate from a Subtitle D landfill, a use that requires only a subset of the model's full capabilities. This manual, then, provides instruction for inexperienced as well as experienced model users who seek to study or design waste disposal facilities.

Rosemarie C. Russo, Ph.D.
Director
Environmental Research Laboratory
Athens, GA

ABSTRACT

The Environmental Protection Agency's Multimedia Exposure Assessment Model (MULTIMED) for exposure assessment simulates the movement of contaminants leaching from a landfill. The model consists of a number of modules which predict concentrations at a receptor due to transport in the subsurface, surface water, or air. This report is an application manual for the use of MULTIMED in modeling Subtitle D land disposal facilities.

When applying MULTIMED to Subtitle D facilities, the landfill, surface water, and air modules in the model are not accessible by the user; only flow and transport through the unsaturated zone and transport in saturated zone can be considered. A steady-state, one-dimensional, semi-analytical module simulates flow in the unsaturated zone. The output from this module, water saturation as a function of depth, is used as input to the unsaturated zone transport module. The latter simulates transient, one-dimensional (vertical) transport in the unsaturated zone and includes the effects of longitudinal dispersion, linear adsorption, and first-order decay. The unsaturated zone transport module calculates steady-state or transient contaminant concentrations. Output from both unsaturated zone modules is used to couple the unsaturated zone transport module with the steady-state or transient, semi-analytical saturated zone transport module. The latter includes one-dimensional uniform flow, three-dimensional dispersion, linear adsorption, first-order decay, and dilution due to direct infiltration into the groundwater plume.

The fate of contaminants in the various media depends on the chemical properties of the contaminants as well as a number of media- and environment-specific parameters. The uncertainty in these parameters can be quantified in MULTIMED using the Monte Carlo simulation technique.

To enhance the user-friendly nature of MULTIMED, a preprocessor, PREMED, and a postprocessor, POSTMED, have been developed. The preprocessor guides the user in the creation of a correct Subtitle D input file by restricting certain options and parameters and by setting appropriate defaults.

This report was submitted in partial fulfillment of Work Assignment Number 32, Contract Number 68-03-3513 by AQUA TERRA Consultants, under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period March 1990 to July 1990, and work was completed as of August 1990.

TABLE OF CONTENTS

Section			Page
Disclaimer			ii
Foreword			iii
Abstract			iv
Figures			ix
Tables			xii
Acknowledgements			xvi
1.0	INTRODUCTION		1
	1.1	Overview of MULTIMED	1
		1.1.1 Model Capabilities	1
		1.1.2 Interaction Framework (AIDE)	3
	1.2	Application of MULTIMED to Subtitle D Land Disposal Facilities	3
	1.3	Report Organization	4
	1.4	How to Use this Manual	4
2.0	PROGRAM INSTALLATION AND EXECUTION		7
	2.1	System Requirements	7
		2.1.1 Hardware	7
		2.1.2 Software	7
	2.2	Loading the Executable Code	7
	2.3	Executing and Verifying Test Sessions	8
3.0	FORMAT AND OPERATION OF THE PRE- AND POSTPROCESSOR		10
	3.1	Screen Format	10
		3.1.1 Data Window	10
		3.1.2 Assistance Window	12
		3.1.3 Instruction Window	16
		3.1.4 Command Line	16
	3.2	Interaction Modes	17
	3.3	Screen Movement	19
		3.3.1 Movement within Screens	19
		3.3.2 Movement between Screens	21
		3.3.3 Screen Path	21
4.0	USE OF THE PRE- AND POSTPROCESSORS		23
	4.1	The Preprocessor (PREMED)	23
		4.1.1 Use of the Preprocessor	23
		4.1.2 The PREMED Tutorials	38
	4.2	The Postprocessor (POSTMED)	39
		4.2.1 Use of the Postprocessor	39
5.0	MODEL APPLICATION		46
	5.1	MULTIMED Capabilities and Limitations	47
		5.1.1 Solution Techniques	47
		5.1.2 Spatial Characteristics of the System	49
		5.1.3 Steady-state Versus Transient Flow and Transport	50
		5.1.4 Monte Carlo Versus Deterministic Simulations	51
		5.1.5 Boundary Conditions	52
	5.2	Subtitle D Applications of MULTIMED	52
		5.2.1 Summary of EPA Requirements for MULTIMED Simulations of Leachate Migration from Subtitle D Facilities	52
		5.2.2 Active Modules	53

5.2.3 Boundary Conditions..... 53
5.2.4 Procedures for Application of MULTIMED to Subtitle D Facility Design..... 53
5.3 MULTIMED Input Requirements..... 56
5.3.1 Parameter Requirements Summarized by Module..... 57
5.3.2 Parameter Requirements Summarized by Data Group... 57

6.0 PARAMETER ESTIMATION..... 77
6.1 Chemical-Specific Parameters..... 78
6.1.1 Overall Chemical Decay Coefficient (Saturated Zone)..... 78
6.1.2 Solid-Phase and Liquid-Phase Decay Coefficients (Saturated Zone)..... 78
6.1.3 The Acid-Catalyzed and Base-Catalyzed Hydrolysis Rates and the Neutral Hydrolysis Rate..... 78
6.1.4 Reference Temperature..... 79
6.1.5 Distribution Coefficient (Saturated Zone)..... 79
6.1.6 Normalized Organic Carbon Distribution Coefficient..... 79
6.1.7 Biodegradation Coefficient (Saturated Zone)..... 80
6.2 Source-Specific Parameters..... 80
6.2.1 Recharge Rate..... 80
6.2.2 Infiltration Rate..... 80
6.2.3 Area of the Waste Disposal Unit..... 81
6.2.4 Length Scale of the Facility..... 81
6.2.5 Width Scale of the Facility..... 81
6.2.6 Initial Concentration at Waste Disposal Facility.. 81
6.2.7 Source Decay Constant..... 81
6.2.8 Duration of Pulse..... 82
6.2.9 Spread of Contaminant Source..... 82
6.3 Unsaturated Flow Parameters..... 82
6.3.1 Saturated Hydraulic Conductivity..... 82
6.3.2 Unsaturated Zone Porosity..... 84
6.3.3 Air Entry Pressure Head..... 85
6.3.4 Number of Layers, Thickness of Layers..... 85
6.3.5 Residual Water Content..... 86
6.3.6 Brooks and Corey Exponent..... 86
6.3.7 Van Genuchten Parameters..... 86

6.4 Unsaturated Transport Parameters..... 87
6.4.1 Number of Layers, Thickness of Layers..... 87
6.4.2 Longitudinal Dispersivity of Each Layer..... 89
6.4.3 Percent Organic Matter..... 89
6.4.4 Bulk Density of Soil for Layer..... 92
6.4.5 Biological Decay Coefficient..... 92
6.5 Aquifer-Specific Parameters..... 92
6.5.1 Aquifer Porosity..... 92
6.5.2 Particle Diameter..... 93
6.5.3 Bulk Density..... 93
6.5.4 Aquifer Thickness..... 95
6.5.5 Source Thickness (Mixing Zone Depth)..... 95
6.5.6 Hydraulic Conductivity..... 98
6.5.7 Hydraulic Gradient..... 99
6.5.8 Groundwater Seepage Velocity..... 99
6.5.9 Retardation Coefficient..... 99
6.5.10 Longitudinal, Transverse, and Vertical Dispersivities..... 100
6.5.11 Aquifer Temperature..... 103
6.5.12 pH..... 103
6.5.13 Organic Carbon Content (Fraction)..... 103
6.5.14 Well Distance from Site, Angle off Center, and Well Vertical Distance..... 103

7.0 EXAMPLE PROBLEMS..... 106
7.1 Example 1..... 106
7.1.1 The Hypothetical Scenario..... 106
7.1.2 Input..... 107
7.1.3 Output..... 110
7.2 Example 2..... 110
7.2.1 The Hypothetical Scenario..... 110
7.2.2 Input..... 110
7.2.3 Output..... 110
7.3 Example 3..... 124
7.3.1 The Hypothetical Scenario..... 124
7.3.2 Input..... 124
7.3.3 Output..... 129

8.0 REFERENCES..... 142

APPENDIX A - CODE STRUCTURE AND INPUT DATA FORMAT..... 148
A.1 Model Structure..... 148
A.2 Input and Output File Units..... 148
A.3 Common Blocks and Parameter Statements..... 151
A.4 Structure of the Input Files..... 154
A.4.1 Comment Cards..... 154
A.4.2 Data Group/Subgroup Specification Card, End Card and Data Cards..... 154
A.4.3 Specification of Parameter Values..... 156
A.4.4 The Array Subgroup..... 157
A.4.5 The Empirical Distribution Subgroup..... 159

A.5 Format of the Data Groups..... 159
A.5.1 General Data Group..... 159
A.5.2 Source Data Group..... 159
A.5.3 Landfill Data Group..... 163
A.5.4 Chemical Data Group..... 168
A.5.5 Unsaturated Flow Data Group..... 170
A.5.6 Unsaturated Transport Data Group..... 184
A.5.7 Aquifer Data Group..... 186
A.5.8 Surface Water Data Group..... 189
A.5.9 Air Emissions and Dispersion Data Group..... 191

APPENDIX B - SUBROUTINES IN MULTIMED..... 201

FIGURES

		Page
2.1	Preprocessor screen after installation.....	8
3.1	Screen format utilized by the pre- and postprocessor.....	11
3.2	Example of a two window, one command line screen.....	12
3.3	Example of a three window, one command line screen.....	13
3.4	Example of a HELP assistance window.....	14
3.5	Example of a LIMITS assistance window.....	15
3.6	Example of information contained in a STATUS assistance window..	16
3.7	Example of an ERROR message in the instruction window.....	17
4.1	Opening screen of the preprocessor.....	23
4.2	Build/Modify screen of the preprocessor.....	24
4.3	Edit screen of the preprocessor.....	25
4.4	Create screen of the preprocessor.....	25
4.5	General-1 screen of the preprocessor.....	26
4.6	General-2 screen of the preprocessor.....	28
4.7	Edit screen of the preprocessor.....	28
4.8	AQuifer screen of the preprocessor.....	29
4.9	SOurce screen of the preprocessor.....	30
4.10	Chemical screen of preprocessor.....	30
4.11	Unsaturated Flow (Funsat) screen of the preprocessor.....	31
4.12	Unsaturated Transport (Tunsat) screen of the preprocessor.....	31
4.13	The Depth screen of the preprocessor.....	32
4.14	The POrosity screen of the preprocessor for a deterministic simulation.....	34
4.15	Screen for specification of aquifer porosity for a deterministic simulation.....	34
4.16	Porosity screen of the preprocessor for a Monte Carlo simulation.....	35

4.17 Screen showing required parameters for a Lognormal probability density distribution..... 35

4.18 The Return screen of the preprocessor..... 37

4.19 The Save screen of the preprocessor..... 37

4.20 Example of a tutorial screen..... 38

4.21 Opening screen of the postprocessor..... 40

4.22 Data-1 screen of the postprocessor..... 41

4.23 Data-2 screen of the postprocessor..... 41

4.24 Specs screen of the postprocessor..... 43

4.25 Titles screen of the postprocessor..... 43

4.26 Example of a cumulative frequency plot..... 44

4.27 Example of a frequency plot..... 44

4.28 Example of screen showing a TEXT file..... 45

5.1 Procedure for using MULTIMED to assist in the design of Subtitle D facilities..... 54

6.1 Schematic of the source thickness and the well location..... 97

6.2 Measured values of longitudinal dispersivity as a function of path length over which dispersion is observed..... 101

6.3 Average temperatures of shallow groundwater in the continental United States..... 104

A.1 Subroutine organization tree for MULTIMED..... 149

A.2 Structure of the input data file, data groups, and subgroups.... 155

A.3 Key options available in the general data group pertaining to the saturated zone transport module..... 164

A.4 Key options available in the surface water module..... 195

A.5 Key options available in the air modules..... 199

TABLES

		Page
3-1	Commands for Application of PREMED	18
5-1	Issues to be Considered before Applying MULTIMED	48
5-2	Primary Parameters Used in the Saturated Zone Transport Module for Subtitle D Applications of MULTIMED	58
5-3	Parameters Used to Derive Other Saturated Zone Transport Module Parameters Needed in Subtitle D Applications of MULTIMED	59
5-4	Parameters Required in the Unsaturated Zone Flow Module for Subtitle D Applications of MULTIMED	61
5-5	Parameters Required in the Unsaturated Zone Transport Module for Subtitle D Applications of MULTIMED	62
5-6	Parameters in the Chemical (Chemical) Data Group	64
5-7	Parameters Required for Selected Probability Density Distributions	67
5-8	Parameters in the Contaminant Source (SOurce) Data Group	68
5-9	Parameters in the Aquifer (AQuifer) Data Group	69
5-10	Parameters in the Unsaturated Zone Flow (Funsat) Data Group	72
5-11	Parameters in the Unsaturated Zone Transport (Tunsat) Data Group	75
6-1	Range of Hydraulic Conductivity Values for Various Geologic Materials	83
6-2	Descriptive Statistics for Saturated Hydraulic Conductivity	84
6-3	Total Porosity of Various Materials	85
6-4	Descriptive Statistics for Saturation Water Content and Residual Water Content	87
6-5	Descriptive Statistics for van Genuchten Water Retention Model Parameters	88
6-6	Compilation of Field Dispersivity Values	90
6-7	Descriptive Statistics and Distribution Model for Organic Matter (Percent by Weight)	91

6-8	Mean Bulk Density for Five Soil Textural Classifications.....	93
6-9	Descriptive Statistics for Bulk Density.....	94
6-10	Range of Soil Particle Sizes for Various Materials.....	95
6-11	Range and Mean Values of Dry Bulk Density for Various Geologic Materials.....	96
6-12(a)	Alternatives for Including Dispersivities in the Saturated Zone Module.....	102
6-12(b)	Probabilistic Representation of Longitudinal Dispersivity for a Distance of 152.4 m.....	102
7-1	Input Sequence for Example 1.....	108
7-2	Output File for Example 1.....	111
7-3	SAT.OUT File for Example 1.....	114
7-4	Input Sequence for Example 2.....	115
7-5	Main Output File for Example 2.....	119
7-6	SAT.OUT File for Example 2.....	123
7-7	Monte Carlo Distribution Values in Example 3.....	124
7-8	Input Sequence for Example 3.....	125
7-9	Main Output File for Example 3.....	130
7-10	First Page of the SAT1.OUT File for Example 3.....	140
7-11	STATS.OUT File for Example 3.....	141
A-1	Input Files Needed in MULTIMED.....	151
A-2	Output Files Generated by MULTIMED.....	152
A-3	Input Data Groups and Subgroups in MULTIMED.....	156
A-4	Distributions Available and their Codes.....	157
A-5	Contents and Format of a Typical Array Subgroup.....	158
A-6	Contents and Format of a Typical Empirical Distribution Subgroup.....	160
A-7	Contents and Format of the General Data Group.....	161
A-8	Example of a Typical General Data Group.....	165
A-9	Contents and Format of the Source-Specific Data Group.....	166
A-10	Variables in the Source-Specific Array Subgroup.....	167
A-11	Contents and Format of the Landfill Module Control Data Group.....	169

A-12 Contents and Format of the Landfill Module Layer Thickness and Material Data Subgroup..... 170

A-13 Contents and Format of the Landfill Module Liner Property Subgroup..... 171

A-14 Variables in the Landfill Liner Property Array Subgroup..... 172

A-15 Contents and Format of the Landfill Module Material Property Subgroup..... 173

A-16 Variables in the Landfill Material Property Array Subgroup... 174

A-17 Contents and Format of the Landfill Module Hydrology Subgroup..... 175

A-18 Variables in the Landfill Hydrology Array Subgroup..... 176

A-19 Contents and Format of the Chemical-Specific Data Group..... 177

A-20 Variables in the Chemical Array Subgroup..... 178

A-21 Contents and Format of the Unsaturated Zone Flow Module Control Data Group..... 179

A-22 Contents and Format of the Unsaturated Flow Module Layer Thickness and Material Data Subgroup..... 181

A-23 Contents and Format of the Unsaturated Zone Flow Module Material Property Subgroup..... 182

A-24 Variables in the Unsaturated Flow Material Property Array Subgroup..... 183

A-25 Contents and Format of the Unsaturated Zone Flow Module Moisture Data Subgroup..... 184

A-26 Variables in the Unsaturated Flow Moisture Data Array Subgroup..... 185

A-27 Contents and Format of the Unsaturated Zone Transport Module Control Data Subgroup..... 187

A-28 Contents and Format of the Unsaturated Zone Transport Module Properties Subgroup..... 189

A-29 Variables in the Unsaturated Transport Properties Array Subgroup..... 190

A-30 Contents and Format of the Aquifer-Specific Data Group..... 191

A-31 Variables in the Aquifer Data Array Subgroup..... 192

A-32 Contents and Format of the Surface Water Data Group..... 193

A-33 Variables in the Surface Water Data Array Subgroup..... 194

A-34 Contents and Format of the Air Emission and Dispersion Data Group..... 196

A-35 Variables in the Air Emission and Dispersion Data Array Subgroup..... 197

A-36 Contents and Format of the Air Dispersion Control Data Subgroup..... 198

A-37 General Structure of the Wind-Stability Frequency File (FREQ.IN)..... 200

ACKNOWLEDGEMENTS

This document was prepared under Work Assignment No. 32 of Contract No. 68-03-3513 by AQUA TERRA Consultants for the U.S. Environmental Protection Agency Office of Research and Development. Gerard Laniak of the Environmental Research Laboratory in Athens, Georgia was the Technical Project Monitor and Robert Carsel was the Project Officer. We thank them for their continuous technical and management support throughout the course of this project.

At AQUA TERRA Consultants, the report was co-authored by Constance Travers and Susan Sharp-Hansen, the Project Manager. Anthony Donigian supplied technical and administrative guidance and he and John Kittle reviewed the document. Word processing was performed by Dorothy Inahara. The material in Appendix A, which summarizes the code structure and input format, and in Appendix B, which lists the model subroutines, is based on a report by Salhotra and Mineart (1988).

A number of individuals were involved in the development and implementation of the MULTIMED computational codes. Key individuals include Jan Kool and Peter Huyakorn of HydroGeoLogic Inc., Terry Allison of Computer Sciences Corporation, Barry Lester of Geotrans Inc., Michael Ungs of TetraTech, Inc., Bob Ambrose of U.S. EPA, John Kittle of AQUA TERRA Consultants, and Rob Schanz, Yvonne Meeks, and Peter Mangarella of Woodward-Clyde Consultants.

The pre- and postprocessor for MULTIMED were developed by John Kittle and Paul Hummel at AQUA TERRA Consultants. Paul Hummel and Constance Travers created the tutorials for the preprocessor.

SECTION 1

INTRODUCTION

This document provides information needed to apply the U.S. Environmental Protection Agency's Multimedia Model (MULTIMED) to scenarios related to the study and design of Subtitle D land disposal facilities. Application of MULTIMED to Subtitle D facilities requires the use of only a subset of the model's capabilities. MULTIMED's model theory documentation (Salhotra et al., 1990) provides detailed information about the model's full capabilities. In this section, the model's full capabilities are first briefly addressed (Section 1.1). A summary of the methods used for application to the design of Subtitle D facilities follows (Section 1.2).

1.1 OVERVIEW OF MULTIMED

MULTIMED simulates the transport and transformation of contaminants released from a waste disposal facility into the multimedia environment. Release to either air or soil, including the unsaturated and the saturated zones, and possible interception of the subsurface contaminant plume by a surface stream are included in the model. Thus, the model can be used as a technical and quantitative management tool to address the problem of the land disposal of chemicals in the multimedia environment. At this time, the air modules of the model are not linked to the other model modules. As a result, the estimated release of contaminants to the air is independent of the estimated contaminant release to the subsurface and surface water.

MULTIMED utilizes analytical and semi-analytical solution techniques to solve the mathematical equations describing flow and transport. The simplifying assumptions required to obtain the analytical solutions limit the complexity of the systems with can be represented by MULTIMED. The model does not account for site-specific spatial variability, the shape of the land disposal facility, site-specific boundary conditions, or multiple aquifers and pumping wells. Nor can MULTIMED simulate processes, such as flow in fractures and chemical reactions between contaminants, which can have a significant affect on the concentration of contaminants at a site. In more complex systems, it may be beneficial to use MULTIMED as a "screening level" model which would allow a user to obtain an understanding of the system. A numerical model could then be used if there are sufficient data and necessity to justify the use of a more complex model.

1.1.1 Model Capabilities

During the development of this model, emphasis was placed on the creation of a unified, user-friendly, software framework, with the capability to perform uncertainty analysis, that can be easily enhanced by adding modules and/or modifying existing modules.

To enhance the user-friendly nature of the model, separate interactive preprocessing and postprocessing software has been developed for use in creating and editing input and in plotting model output. The pre- and postprocessors, PREMED and POSTMED, have not been integrated with MULTIMED because of the size limitations of PC computers. Therefore, after using the preprocessor to create or modify input, the model is run in batch mode. Afterwards, the postprocessor can be used to produce plots of the Monte Carlo output or plots of concentration versus time for transient output.

The fate of contaminants critically depends on a number of media-specific parameters. Typically many of these parameters exhibit spatial and temporal variability as well as variability due to measurement errors. MULTIMED has the capability to analyze the impact of uncertainty and variability in the model inputs on the model outputs (concentrations at specified points in the multimedia environment), using the Monte Carlo simulation technique.

The major functions currently performed by this model include:

- Allocation of default values to some input parameters/variables.
- Reading of the input data files.
- Echo of input data to output files.
- Derivation of some parameters, if specified by the user.
- Depending on user-selected options:
  - simulation of leachate flux emanating from the source
  - simulation of unsaturated zone flow and transport
  - simulation of saturated zone transport only
  - computation of in-stream concentrations due to contaminant loading assuming complete interception of a plume in the saturated zone
  - computation of the rate of contaminant emission from the waste disposal unit into the atmosphere
  - simulation of dispersion of the contaminants in the atmosphere
- Generation of random input values for Monte Carlo simulations.
- Performance of statistical analyses of Monte Carlo simulations.
- Writing the concentrations at specified receptors to output files for deterministic runs. In the Monte Carlo mode, writing the cumulative frequency distribution and selected percentiles of concentrations at receptors to output files.
- Printing the values of randomly generated input parameters and the computed concentration values for each Monte Carlo run.

1.1.2 Interaction Framework (AIDE)

The pre- and postprocessor for MULTIMED have been developed using the ANNIE Interaction Development Environment (AIDE) (Kittle et al., 1989). Consequently, the construction of input and the analysis of output is standardized in terms of screen formats, movement within and between screens, and methods of entering data, seeking on-line assistance and invoking commands. A full explanation of the conventions used is provided in Section 3.

1.2 APPLICATION OF MULTIMED TO SUBTITLE D LAND DISPOSAL FACILITIES

The U.S. EPA has developed several restrictions for Subtitle D applications of MULTIMED. These restrictions were made in an effort to develop a conservative approach for simulating leachate migration from Subtitle D facilities.

- Only the Saturated and/or Unsaturated Modules may be active in Subtitle D applications, because the Surface Water, Landfill and Air Modules have not been sufficiently tested at this time.

- Although MULTIMED can simulate either steady-state or transient transport conditions, only steady-state transport simulations are allowed for Subtitle D applications. No decay of the source term is allowed; the concentration of contaminants entering the aquifer system must be constant in time. The contaminant pulse is assumed continuous and constant for the duration of the simulation.

- The receptor must be located directly downgradient of the facility, so that it intercepts the center of the contaminant plume. In addition, the contaminant concentration must be calculated at the top of aquifer. Therefore, the angle from the plume centerline to the receptor and the vertical distance to the receptor must be specified as zero in Subtitle D applications.

Thus, MULTIMED can be applied at many Subtitle D land disposal facility sites to simulate the transport of contaminants from the source, through the saturated and/or unsaturated zones by groundwater, to a receptor (i.e. a well). When MULTIMED is used in conjunction with a separate source model, such as HELP (Schroeder et al., 1984), it can be used in a variety of applications. These applications include 1) development and comparison of the effects of different facility designs on groundwater quality, 2) prediction of the results of different types of "failure" of the landfill, and 3) if leachate migration into the groundwater below an existing waste disposal facility occurs, prediction of the fate and transport of the contaminants in the subsurface. The user should bear in mind, however, that MULTIMED may not be an appropriate model for application to some sites. This issue, which is discussed in Section 5.1, should be considered before modeling efforts proceed.

As stated above, MULTIMED can be used in the design process to demonstrate that a particular design will adequately prevent contaminant concentrations in groundwater from exceeding health-based thresholds. In other words, MULTIMED combined with a source model can be used to demonstrate that either a landfill design, or the specific hydrogeologic conditions present at a site will prevent the migration of significant quantities of contaminants from the landfill. Procedures have been developed for the application of MULTIMED to the design of Subtitle D facilities. These procedures are outlined in Section 5.2.4 and are briefly summarized here.

- Collect site-specific hydrogeologic data

- Determine the contaminant to be simulated and the active modules in MULTIMED and the point of compliance

- Propose a landfill design and determine the corresponding

infiltration rate

- Run MULTIMED and calculate the dilution attenuation factor (i.e., the factor by which the concentration is expected to decrease between the landfill and the point of compliance)

- Based on the resulting dilution attenuation factor, determine if the design is acceptable

1.3 REPORT ORGANIZATION

This report contains the information needed to apply MULTIMED, in conjunction with another model, such as HELP (Schroeder et al., 1984 a and b), to Subtitle D land disposal facilities. Section 2 contains information about installation and execution of the code. In Section 3, general information about the format and operation of the pre- and postprocessors is provided and Section 4 describes how to use the pre- and postprocessors for Subtitle D applications of the model. Section 5 discusses the development of a conceptual model for Subtitle D applications, the limitations and capabilities of MULTIMED, and details about the input required to run each model module. Help in estimating some of the model parameters is contained in Section 6. In Section 7, appropriate example problems are included. Finally, contained in Appendices are 1) detailed information on the structure of the code and the format of data in the input files, and 2) a listing of the subroutines in the code.

1.4 HOW TO USE THIS MANUAL

This application manual for the MULTIMED model and its pre- and postprocessors, PREMED and POSTMED, is designed to be used by inexperienced as well as experienced users. Instructions are suggested for two types of inexperienced users: the "hands-on, learn-as-you-go" user and the "read the document first" user, as well as for the experienced user. An experienced user is defined as one who is already familiar with the basic capabilities and operational aspects of PREMED, MULTIMED and POSTMED, and wants to use the programs to perform simulations. These instructions are based on a similar set of instructions found in Imhoff et al. (1990).

"Hands-on, Learn-as-you-go" Users

1. Read Section 2 for instructions on model installation and execution.

2. Install PREMED, MULTIMED, and POSTMED. Execute the tests provided with the code and/or described in Section 2 to verify that PREMED and POSTMED are properly installed.

3. From the DOS operating system, execute PREMED by typing <PREMED> (do not type the brackets). The opening screen will appear. Utilize one of the two tutorials by typing either <@DETER.LOG> for a deterministic Subtitle D application or <@MONTE.LOG> for a Monte Carlo Subtitle D application.

4. Use the completed input sequence generated by the selected tutorial to run MULTIMED. The input sequence created by the <@DETER.LOG> tutorial is the same as that used in Example 2 in Section 7. The input generated by the <@MONTE.LOG> tutorial corresponds to Example 3 in Section 7.

5. Examine the output generated by the MULTIMED model. Because new versions of MULTIMED may be released after publication of this document, the output may not be identical to the output shown in Section 7. Therefore, compare the output generated by MULTIMED with the appropriate output file provided with the code. This will allow you to verify that the MULTIMED model is properly installed.

6. Try the other example problems described in Section 7 to become more familiar with MULTIMED.

7. Practice producing plots using POSTMED and the SAT1.OUT file generated when the Example 3 input is run.

8. Proceed with suggestions 2 through 5 provided below for "experienced users."

"Read the Documentation First" Users

1. Read Section 1 to familiarize yourself with the basic capabilities and framework of the MULTIMED model. If you need more detailed information on the capabilities and limitations of MULTIMED to determine if the model will be suitable for your needs, read Section 5.1.

2. Read Section 3 which discusses the format and basic operation of the preprocessor, PREMED.

3. Read Section 2 for instructions on model installation and execution.

4. Install PREMED, MULTIMED, and POSTMED. Execute the tests provided with the code and/or described in Section 2 to verify that PREMED and POSTMED are properly installed.

5. From the DOS operating system, execute PREMED by typing <PREMED> (do not type the brackets). The opening screen will appear. Utilize one of the two tutorials by typing either <@DETER.LOG> for a deterministic Subtitle D application or <@MONTE.LOG> for a Monte Carlo Subtitle D application.

6. Section 4 discusses the use of the pre- and post-processor. Read Section 4.1 in conjunction with the tutorial to provide a complete description of PREMED.

7. Use the completed input sequence generated by the selected tutorial to run MULTIMED. The input sequence created by the <@DETER.LOG> tutorial is the same as that used in Example 2 in Section 7. The input generated by the <@MONTE.LOG> tutorial corresponds to Example 3 in Section 7.

8. Examine the output generated by the MULTIMED model. Because new versions of MULTIMED may be released after publication of this document, the output may not be identical to the output shown in Section 7. Therefore, compare the output generated by MULTIMED with the appropriate output file provided with the code. This will allow you to verify that the MULTIMED model is properly installed.

9. Try the other example problems described in Section 7 to become more familiar with MULTIMED.

10. Practice producing plots using POSTMED and the SAT1.OUT file generated when the Example 3 input is run.

11. Proceed with suggestions 2 through 5 provided below for "experienced users."

Experienced Users

1. Read Section 2 and install PREMED, MULTIMED, and POSTMED. Execute the tests provided with the code and/or described in Section 2 to verify that PREMED and POSTMED are properly installed, and execute the test run for PREMED.

2. Read Section 5.2 which discusses applying MULTIMED to Subtitle D facility problems. Refer to Section 5.1, which includes a discussion of issues related to conceptualization of the system, and the capabilities and limitations of MULTIMED, as needed.

3. Read Section 6 as needed to estimate parameters required by MULTIMED.

4. Try using MULTIMED to simulate actual scenarios.

5. If you wish to make changes to input files without using the preprocessor, refer to Appendix A which discusses the format for input files.

SECTION 2

PROGRAM INSTALLATION AND EXECUTION

This section describes how to install and test MULTIMED and the related pre- and postprocessor software on the user's computer. Hardware and software requirements are discussed. Exact details of installation are included with the software when it is distributed by the EPA Center for Exposure Assessment Modeling (CEAM) at the Environmental Research Laboratory in Athens, Georgia. If problems are experienced, the user should contact CEAM for support.

2.1 SYSTEM REQUIREMENTS

2.1.1 Hardware

MULTIMED and the related pre- and postprocessors, PREMED and POSTMED, were designed to be used on an IBM-PC compatible computer. The PC must have 640 KB of memory, a math coprocessor, and approximately 4 MB of free disk space.

Additional machines which should run the software include Digital Equipment Corporation VAX computers running the VMS operation system, Prime 50 Series computer running PRIMOS and Sun Microsystems workstations running UNIX. Contact CEAM for details.

2.1.2 Software

MULTIMED and its related software are written in FORTRAN 77. If compilation of the code is required, a FORTRAN compiler and linker are needed. In addition, compilation of the preprocessor, PREMED, and postprocessor, POSTMED, requires the use of ANNIE-IDE software (Kittle et al., 1989), which is available from CEAM. Graphics in the model postprocessor use the ANSI Graphical Kernel System (GKS). If the graph features of the postprocessor are to be used, then GKS device drivers are required for the user's output and input devices. Consult CEAM for additional information about obtaining these device drivers.

2.2 LOADING THE EXECUTABLE CODE

Included with the distribution media for MULTIMED and its related pre- and postprocessing software is a README.1ST document and file that provides detailed instructions for installing the programs. It is recommended that data files be maintained in directories separate from the code.

2.3 EXECUTING AND VERIFYING TEST SESSIONS

Sample input data files and the related output files are distributed with the model. In order to test the installation of MULTIMED, the user should run these example problems and compare the output generated by the code with the output files supplied with the code. The code is executed on a PC by typing **MULTIMED<CR>** (<CR> is the enter key). The model will query the user for the name of the input file and the name of the file to which output should be written. Be careful not to overwrite existing output files.

In order to test the installation of the preprocessor, perform the following check. First, execute the program (on a PC type **PREMED<CR>**). Next type the following sequence of keys:

BCS<CR><CR>M<F2><F2>FU<F2>RRYRY

Note that **<F2>** is the F2 function key. The screen in Figure 2.1 should appear on the display screen. To return to the operating system, type the key **R**.

The best test of the installation of the postprocessor is to plot the results of the Monte Carlo simulation distributed with the model. The output file is called EX3SAT1.OUT. First, execute the program (on a PC type **POSTMED<CR>**). Next, for plotting results to the screen type the following sequence of keys:

D<F2>EX3SAT1.OUT<F2>P

A cumulative frequency plot will appear on the computer screen. This plot should be the same as the cumulative frequency plot found in the main output file for the same problem. After examining the plot, press the Escape key, **Esc**, to clear the plot from the screen. To return to the operating system, type the key **R**.

For computers without graphics capabilities, the following check can be performed. After executing the program (on a PC type **POSTMED<CR>**), type the following sequence of keys:

D<F2>EX3SAT1.OUT<F2>S

At this point, hit the down arrow key once, then type **PR<F2>P**. The cumulative frequency plot will be sent to the printer. After the plot has been sent, return to the operating system by typing the key **R**.

If there is a problem with any of the three software components of MULTIMED, review the installation instructions carefully before calling CEAM for support.

SECTION 3

FORMAT AND OPERATION OF THE PRE- AND POSTPROCESSOR

A pre- and a postprocessor, PREMED and POSTMED, have been developed for MULTIMED in order to improve the ease with which input can be created and/or edited and output can be analyzed. The pre- and postprocessors have been developed using the ANNIE Interaction Development Environment (Annie-IDE) (Kittle et al., 1989). Consequently, user interaction within the program is standardized in terms of screen formats, movement within and between screens, and methods of entering data, seeking on-line assistance and invoking commands.

Two tutorials are distributed with the preprocessor (see Section 4.1.3 for information about running the tutorials). These tutorials familiarize the user with the operation and features of the preprocessor and are recommended for new users. Although no tutorial exists for the postprocessor, its format and operation are identical to that of the preprocessor. To complement the tutorials, the format and operation of the screens are described in detail below. The summary is taken, with minimal adaptation, from the manual for another Annie-IDE application, called DBAPE (Imhoff et al., 1989).

3.1 SCREEN FORMAT

Figure 3.1 defines the basic layout of a preprocessor screen. The layout is consistent for all screens used by PREMED, with specific kinds of information always located at the same region of the screen. Screen information is divided into four components: three windows (data window, assistance window, instruction window) and the command line. For convenience, the dimensions, content, and important features of the four screen components are summarized along the periphery of the screen area in the figure.

3.1.1 Data Window

The top portion of the screen is the **data window.** The data window contents consist of one or more of the following.

(1) Prompts for user-supplied decisions by means of menu selection

(2) Prompts for user-supplied data by means of form fill-in

(3) Echoes for current state of data

Two user-controlled sizes for the data window are used. In the default layout, the assistance window is not displayed, resulting in a two window, one commandline screen (see Figure 3.2 for example). If the user desires any of the forms of assistance described in Section 3.1.2, then the data window is reduced in size to accommodate the assistance window (see Figure 3.3).

Conversely, the assistance window can be eliminated from the screen, thus expanding the data window, by invoking the QUIET command (**<F8>**). The pre- and postprocessors accommodate up to 50 lines of data and enable scrolling in the data window by using cursor keys when the data size exceeds the window size. The title of the window and a series of one letter codes which identify the sequence of screens which have led up to the current screen is displayed on the upper left hand border of the data window. Further explanation of the "screen path" feature is provided in Section 3.3.3.

3.1.2 Assistance Window

Several types of user assistance are available within the pre- and postprocessors. A layered approach to assistance is used as follows.

(1) Use of descriptive and unique words or abbreviations for field or menu option names in the data window always provides "first-cut" definitions.

(2) When space allows, additional information in the data window near the data field or menu option clarifies the desired information.

(3) If additional parameter- or screen-specific assistance is available, it is supplied, upon request by the user, in the assistance window. Two types of screen-dependent assistance can be displayed in the assistance window: HELP and LIMITS.

(4) If assistance of a global nature (i.e., independent of individual screens) is available, it, also, is displayed in the assistance window upon request by the user. The three types of global assistance which can be displayed in the assistance window are CMND, STATUS and XPAD.

The layered "help" in PREMED and POSTMED is designed so that the user must specifically request the higher levels of assistance; consequently, experienced users are not subjected to unnecessary information.

As specified above, the **assistance window**, which is located directly below the data window (Figure 3.1), is used to display the more detailed levels of assistance (HELP, LIMITS, CMND, STATUS and XPAD). All types of detailed assistance are further described later in this section. The user selects one assistance type at a time and the available assistance of that type is displayed in the assistance window. The title of the window (i.e., HELP, LIMITS, CMND, STATUS or XPAD) is displayed on the left portion of the upper border for the window and corresponds to the type of assistance which has been requested by the user. The types of assistance which are available for a particular screen are indicated by the options listed in the command line (Section 3.1.4). If the amount of available assistance exceeds the window size, scrolling in the window by using cursor keys is allowed.

An example of screen layout for a three-window screen is shown in Figure 3.3. Details on each of the assistance types which may be displayed within the assistance window follow.

HELP

HELP assistance provides further information on model and system parameters and menu options (see Figure 3.4). As noted above, HELP text is specific to a particular screen and can be scrolled in the assistance window.

LIMITS

LIMITS displays the allowable values for a specific field in the data window. LIMITS information may be (1) maximum and minimum acceptable numeric values or (2) a list of acceptable alphanumeric values. LIMITS text is specific to the field currently highlighted in the data window, and it, also, can be scrolled. Figure 3.5 shows the type of information displayed in the assistance window when LIMITS has been selected.

CMND

CMND displays the names and definitions of all active commands at the current location. The command definitions never change. It should be noted, however, that the list of available commands varies according to location within the program. For example, the STATUS command is available only at certain program "levels." CMND text can be scrolled in the assistance window.

STATUS

STATUS assistance displays system status messages that summarize previous actions and indicate the relative location of the user within the program structure. A maximum of 10 lines of STATUS assistance may be viewed by the user at any point within an application; STATUS assistance cannot be scrolled. Figure 3.6 illustrates the type of information displayed in the STATUS message. The screen contains the following information.

(1) Whether a file is being created or edited. If editing an existing file, the file name is given.

(2) The type of application (i.e., a generic model application or a Subtitle D application).

(3) The scenario being modeled (i.e., the MULTIMED modules which have been selected by the user).

XPAD

Scratch pad (XPAD) assistance allows the user to write notes and reminders during an interactive session. The user may record information in a single XPAD with a maximum width of 78 characters and length of 10 lines. Regardless of where the user is located within the interactive session, a request for XPAD assistance will call up the same XPAD with the same information. XPAD information in the assistance window can be scrolled. New notes can be added to existing notes, and existing notes can be overwritten.

3.1.3 Instruction Window

The **instruction window** is always present on every screen. In the screen layout, it is located below the data and assistance windows and directly above the command line (see Figure 3.1). Two types of information are provided in the window: instructions for the user's next keystroke or error messages reporting incorrect keystrokes with instructions for corrective actions. Depending on which type of information is displayed by the system, the window title on the screen will be either "INSTRUCT" or "ERROR." Figure 3.5 gives an example of the type of information commonly provided in an INSTRUCT-type instruction window, and Figure 3.7 illustrates an ERROR-type instruction window.

3.1.4 Command Line

The final component of the standard pre- and postprocessor screen is the **command line** (Figure 3.1). The command line is restricted to one line. It contains a menu of abbreviations for the available commands at the user's current location within the program structure. Definitions of the abbreviated commands are available by invoking the CMND assistance in the assistance window.

Table 3.1 lists the commands available in PREMED, the function keys used to invoke commands, and command definitions. Inspection of the command line in Figure 3.1 shows that some of the commands are associated with the PC functions keys and some are not. Instructions on the alternate methods for invoking the various commands are provided in Section 3.3.

A final feature of the command line is mentioned here to avoid confusion. As

will be explained in the following section, three interaction modes can be utilized: data mode, command mode, and assist mode. The command line appears on the screen when the user is utilizing either the data mode or the command mode. When the user has invoked the assist mode, the command line is removed from the screen to avoid confusion, and command instructions are displayed in the instruction window. When the user leaves the assist mode to return to either of the other two modes, the command line reappears.

3.2 INTERACTION MODES

User interaction is organized into three "modes," each with a specific function:

(1) Use **data mode** to enter data or select from menu options in data window.

(2) Use **command mode** to invoke commands or functions listed in the command line; commands perform three functions:

  (a) Allow exit from screens (NEXT, PREV).
  (b) Manage assistance window (HELP, LIMITS, XPAD, STATUS, CMND, QUIET).
  (c) Manipulate data window (OOPS).

(3) Use **assist mode** to provide supplemental information in the scratch pad (XPAD) on which to base subsequent actions or to scroll up or down in the assistance window.

Note that most tasks performed will only require use of the data and command modes.

TABLE 3-1. COMMANDS FOR APPLICATION OF PREMED

Command Name	Function Key	Command Definition
CMND		Display definitions of commands in assistance information window
DNPG		Display next page in data window.
HELP	<F1>	Display HELP information in assistance information window
LIMITS	<F5>	Display limits of current field in assistance information window
NEXT	<F2>	Go to next screen (sets screen exit status code to 1)
OOPS		Reset data values in data window to values when screen was first displayed
PREV	<F4>	Go to previous screen
QUIET	<F8>	Turn off assistance information window to allow more room for data
STATUS	<F7>	Display system status in assistance information window
XPAD	<F9>	Display users scratch pad, allow changes

Movement from each of the interaction modes to the other modes can be accomplished as follows.

data mode to **command mode**	- press **<esc>** key
data mode to **assist mode**	- press function key associated with appropriate type of assistance **or** enter command mode and select appropriate assistance from options in command line
command mode to **data mode**	- press **<esc>** key
command mode to **assist mode**	- select appropriate type of assistance from options in command line
assist mode to **data mode**	- press **<esc>** key
assist mode to **command mode**	- press **<esc>** key twice (goes through data mode)

3.3 SCREEN MOVEMENT

Commands may be invoked either by pressing designated function keys or by typing the first letter of a command name. Likewise, menu options may be selected either by moving the cursor to the selection field and confirming, or by typing the first letter (or letters, if needed) of the menu item.

Several general features of user communication should be noted:

(1) There are no restrictions to upper- or lower-case mode.

(2) A key or command is always used to invoke the same function.

(3) Function keys are only used to invoke commands.

3.3.1 Movement Within Screens

Movement within screens may consist of (1) movement between interaction modes, (2) movement between the three windows and the command line, or (3) movement within a window or command line. The first type of movement, between interaction modes, has already been described in Section 3.2 and will not be further considered here. Procedures which cause movement within and between the three windows and the command line of a screen are outlined below. For organization, the procedures which cause movement are categorized in terms of the three interaction modes.

Data Mode--

In data mode, screen movement and operations may be accomplished by pressing either printable character keystrokes, the **<enter>** or **<return>** key, the cursor keys or selected function keys. However, the result of pressing some of these keys depends on the type of screen which is presently displayed.

If one is prompted for decisions by means of a menu (i.e., a **menu screen**), keystrokes cause the following results.

(1) **Type** the first letter (or more, if needed) of any option in the menu in order to select the option.

(2) **Use** cursor keys to move between highlighted menu options.

(3) **Press** function keys designated on the command line to invoke the following commands.

<F1> - HELP **<F2>** - NEXT **<F4>** - PREV **<F9>** - XPAD

If one is prompted for data by means of form fill-in (i.e., a **data screen**), keystrokes cause the following results.

(1) **Type** alphanumeric characters needed to correctly fill in the data screen; the characters will be inserted in the screen at the cursor position.

(2) **Press <enter>** or **<return>** to end entry in one data field and move to another.

(3) **Use** cursor keys to move within and among data screen fields as needed.

(4) **Use** function keys to invoke the following command functions.

<F1> - HELP **<F2>** - NEXT **<F4>** - PREV **<F5>** - LIMITS
<F9> - XPAD

Command Mode--

In the command mode, three categories of keystrokes cause movement within screens.

(1) All commands, with the exception of NEXT and PREV (see Section 3.3.2), cause movement within screens. **Type** the first character of any of these commands to invoke the command and cause activity in either the data or the assistance window. The activity caused by invoking each command is summarized in Table 3-1. As described in Section 3.1.2, the commands CMND, HELP, LIMITS, STATUS, QUIET and XPAD cause activity in the assistance window. The command OOPS, which resets values in data screen to the values present when the screen was first displayed, causes activity exclusively in the data window.

(2) **Press** the **<enter>** or **<return>** key to execute the command currently highlighted in the command line.

(3) **Use** the right or left cursor keys to move the highlighting to another command along the command line.

Assist Mode--

While the user is in the assist mode, keystrokes cause no actions whatsoever unless (1) the scratch pad (XPAD) is active or (2) information which can be scrolled is contained in the assistance window. If the scratch pad is active, typed characters are inserted into the scratch pad at the current location of the cursor. The cursor can move in all directions, and pressing the **<enter>** or **<return>** key causes the start of a new line. Cursor keys can be used to scroll up or down in any assistance window when the available assistance exceeds the window height.

3.3.2 Movement Between Screens

A user can leave one screen and move on to another either by (1) selecting a menu option in the data window or (2) invoking commands displayed on the command line.

Menu Options--

Selection of a menu option always leads to a new screen. From the data mode, menu selections can be made by one of two methods.

(1) **Type** the first letter (or letters, if needed) of the menu item.

(2) **Move** the cursor by use of cursor keys to the selection field and confirm by typing **<esc> N**.

Command Options--

Invoking either the NEXT or the PREV command results in movement to another screen. From the command mode, command selections can be made by one of three methods.

(1) **Type** the first letter of the command.

(2) **Move** the cursor by use of cursor keys to the selection field in the command line and confirm by pressing **<enter>**.

(3) For commands which are associated with a function key (as indicated in the command line), **press** the appropriate function key.

3.3.3 Screen Path

During an interactive session, an aid is provided for remembering the sequence of screens which have led up to the screen which is currently being displayed. The **screen path** is connoted along the upper left hand border of the data window following the window title (see Figure 3.7). The screen path is a series of one or two letter codes which identify both (1) the type of operations and (2) the sequence of operations which have occurred from the time the user leaves the opening screen until arriving at the current screen. For example, a screen path "BCS" in the preprocessor signifies that the current screen is a result of (1) selecting the **B**uild option on the opening screen, (2) opting to **C**reate a new input file, and (3) selecting a **S**ubtitle D application.

As the user branches downward, a letter is added to the screen path each time an operation is performed which results in the display of a new screen. The letter corresponds to the first letter of the option selected in the previous screen. In the case of some menus two letters are needed to differentiate between options. In such cases, both letters are added to the screen path. Conversely, upward movement, which is accomplished by using the **R**eturn option in any menu, results in the elimination of a letter from the screen path.

It should be noted that familiarity with screen sequencing can also speed up the time it takes to perform frequent tasks. After memorizing the screen path needed to perform a sequence of operations and, hence, arrive at a particular location in the program, one may type ahead and pass quickly over intermediate screens.

SECTION 4

USE OF THE PRE- AND POSTPROCESSORS

The preprocessor, PREMED, allows the user to easily create an input file for use in MULTIMED. The postprocessor, POSTMED, provides a means of generating graphs of concentration versus time and the results of Monte Carlo analysis. Both of these programs are designed to be fully interactive and easy to use. Many of the features and options available in the pre- and postprocessors are discussed in Section 3.

4.1 THE PREPROCESSOR (PREMED)

4.1.1 Use of the Preprocessor

Before using the preprocessor, read the section on installation and execution of MULTIMED (Section 2).

To execute the preprocessor, move to the directory which contains the preprocessor and type <PREMED> (do not type the brackets). After a moment the **Opening screen** will appear, as shown in Figure 4.1.

If you are unfamiliar with PREMED, it is strongly recommended that you utilize the tutorials which are included with the preprocessor. These tutorials can be accessed from the **Opening screen** by typing either <@DETER.LOG> or <@MONTE.LOG> (do not type the brackets). The tutorials are discussed in Section 4.1.3.

The **Opening screen** displays several options. At this time, only the **Build/Modify** and **Return** (to operating system) options can be used. Currently it is not possible to analyze model results or execute MULTIMED from the preprocessor. You can analyze the results from Monte Carlo simulations using the postprocessor, POSTMED. Viewing results or executing MULTIMED requires that you return to the operating system.

You must use the **Build/Modify** option to create or edit an input file for MULTIMED. Select this option by typing <B> (do not type the brackets). The **Build/Modify** screen will now be displayed as shown in Figure 4.2.

From this screen, you may either create, edit, or save an input sequence for use in MULTIMED. If you select the **Edit** option (by typing <E>) you will be prompted for the name of a preexisting input file (Figure 4.3). Type the name of a file, and select the "Next" option by pressing <F2> to continue with the program.

If you select the **Create** option, the **Create** screen will be displayed. Figure 4.4 shows the **Create** screen. This screen displays options for either a Generic or a Subtitle D application of MULTIMED. Only Subtitle D applications are discussed in this manual. Since it is intended for regulatory application,the Subtitle D application of MULTIMED restricts the options available for simulation to those which have been thoroughly tested. Therefore, only the scenario involving the Unsaturated Zone and Saturated Zones may be executed, and the Landfill, Surface Water, or Air Modules may not be used. Furthermore, the Subtitle D-specific applications may only be run in steady-state mode.

The next screen which will be displayed by PREMED is the **General-1 (BEG)** screen. This screen allows input of information in the General Data group. Figure 4.5 shows the appearance of the **General-1** screen when the user has chosen to create a Subtitle D input sequence. If a Generic application is selected on the **Create** screen, then the default values on the **General-1** screen

will be different.

The **Run Title** is allowed a maximum of two lines. You may use any title for your simulation that you want. In Subtitle D applications, the **Run Option** may be either deterministic or Monte Carlo, but the simulation must be run in steady-state. Factors which should be considered when selecting these options are discussed in Section 5.

The various modules in MULTIMED which will be active in the simulation must be selected. The Subtitle D application may include only the Saturated Zone and/or Unsaturated Zone Modules. The Saturated Zone Module should be used alone only if the water table is located directly below the bottom of the waste disposal facility. In all other cases, the effects of unsaturated flow and transport from the bottom of the facility to the water table cannot be considered negligible, and the Unsaturated Zone Modules should be included in the simulation. At this time, the other modules shown in Figure 4.5 (Surface water, Air and Landfill) have not been sufficiently tested. Subtitle D applications must be run in steady-state. After the **General-1** parameters have been specified, press <F2> for "Next" to move to the next screen.

If the Monte Carlo option is selected, the **General-1 (BEG)** screen will be followed by the **General-2 (BEG)** screen (Figure 4.6). This screen requires the following input: the number of Monte Carlo simulations, the desired output from the model, and the confidence level (in %) for the 80th, 85th, 90th and 95th estimated percentiles. Estimation of the number of Monte Carlo simulations and confidence levels are discussed in Section 6.6. The amount of output is related to the number of output files which are opened by the model:

LOTS- Opens all ".VAR" and ".OUT" files (i.e., writes the Monte Carlo variables for each simulation and the corresponding output) and the main output file.

SOME- Opens only the main output file, "STATS.OUT" and "SAT1.OUT".

NONE- Opens only the main output file and "STATS.OUT". Note that the postprocessor cannot be used if this amount of output is selected, since POSTMED requires the "SAT1.OUT" file for the simulation.

After the **General-2 (BEG)** screen parameters have been set as desired, press the <F2> to move to the next screen.

The **Edit (BE)** screen will now be displayed as shown in Figure 4.7. This screen allows access to the nine data groups included in MULTIMED: the **General, AQuifer, Air, SOurce, SUrface, Chemical, Funsat, Landfill** and **Tunsat** data groups. Not all of these data groups are required for a specific simulation. For example, if the Air Module was not selected as an active module on the **General-1 (BEG)** screen, then the **Air** data group option on the **Edit (BE)** screen does not need to be selected. To determine which parameters are required for a particular scenario (i.e., combination of MULTIMED modules), refer to the section in the MULTIMED model theory documentation (Salhotra et al., 1990) which describes the module.

The parameters in the **General** data group have already been specified on the **General-1** (and **General-2**) screens. However, if you wish to make changes to this data group, type <G> to select this option.

The **Undef** option on the **Edit (BE)** screen lists the data groups which contain undefined parameters. This option is selected by typing <U>. The data groups displayed contain undefined parameters which will need to be defined before the input sequence is complete for use in MULTIMED. To return to the **Edit** screen, press the <F2> function key.

The other data group options on the **Edit (BE)** screen can be selected by typing enough characters to make the selection unique. For example, there are two

options which begin with "A", so if you wish to select the **AQuifer** data group, you must type <AQ>. Selection of a data group will be followed by a screen which is specific to that data group, and contains a list of parameters or parameter groups which are contained in that data group.

Six data groups contain parameters which are used in simulations of Subtitle D facilities: **General, AQuifer, SOurce, Chemical, Funsat** and **Tunsat.** The **General** data group has already been discussed. The data group-specific screens for each of the other groups are shown in Figures 4.8 through 4.12. Each of these screens contains a **Return** (to **Edit** screen) option, and an option to list **Undef**ined parameters within the data group. **Undef**ined parameters are those which do not have a data value assigned to them. They are designated by a -999 in the input file.

The rest of the options shown in the data-group specific screens are either 1) parameter names or 2) sub-data groups which contain additional parameters. For example, selection of the **Type** option on the **AQuifer** screen (Figure 4.8) will be followed directly by a screen where a parameter value is specified. In this case, the **Type** of source for the saturated zone model is specified. However, selection of the **Depth** option on the **AQuifer** screen will be followed by another screen which contains several parameters related to the size and particle characteristics of the aquifer: **PArticle diameter, POrosity of aquifer, Bulk density, Depth of aquifer** and **Mixing zone depth.** You will need to select one of these options to specify actual values for the parameters. Any of the options may be selected by typing enough characters to make the selection unique.

The specification of a parameter value is similar for all of the parameters in the data groups. Therefore, specification of the aquifer porosity will be used as an example. The other parameters can be specified in a similar manner.

From Table 5-8, it can be determined that the aquifer porosity is part of the **Depth and Particle Characteristics** sub-data group which is part of the **AQuifer** data group. Therefore, the **AQuifer** option should be selected from the **Edit (BE)** screen by typing <AQ>. PREMED will now display the **AQuifer (BEAq)** screen as shown in Figure 4.8. This screen contains five sub-data groups: the **Depth, Type, Hydraulic, Misc** and **Times** data groups. The aquifer porosity is included in the **Depth** (and particle characteristics of the aquifer) sub-data group. Select this option by typing <D>.

The **Depth (BEAqD)** screen will now be displayed. Figure 4.13 shows this screen which contains five parameters for which values may be specified: the **PArticle, POrosity, Bulk, Depth,** and **Mixing.** Select the **POrosity** option on the **Depth (BEAqD)** screen by typing <PO>. The screens which follow this selection will differ for the Deterministic and Monte Carlo simulations. Both types of simulations are discussed below.

Deterministic simulation:

Some of the parameters in MULTIMED may be derived from other parameters instead of being specified directly by the user. The aquifer porosity is one of these parameters which can be derived. Therefore, the **Depth** screen is followed by the **POrosity (BEAqDPo)** screen, shown in Figure 4.14, which provides two options: 1) **Derive** the aquifer porosity value from other parameters in MULTIMED or 2) **Specify** the value of the aquifer porosity. If the **Derive** option is selected, PREMED will return to the **Depth (BEAqD)** screen. However, if the **Specify** option is chosen, the preprocessor will display the screen shown in Figure 4.15. The value of the aquifer porosity should be entered on this screen. After the porosity has been specified, press <F2> to return to the **Size** screen.

Monte Carlo simulation:

The screens which will be displayed for a Monte Carlo simulation are identical to those for a deterministic simulation until the value for a specific parameter is to be input. In a Monte Carlo simulation, the probability density distribution for each parameter required by MULTIMED must be specified.

In the example discussed above, when the **POrosity** option is selected from the **Depth (BEAqD)** screen, the screen which follows is shown in Figure 4.16. The probability density distribution for the **POrosity** is specified on this screen. It is very important that the distribution selected adequately reflects the actual probability density distribution for the parameter. A discussion of probability density distributions is included in the MULTIMED model theory documentation (Salhotra et al., 1990).

Each of the distributions requires that some characteristics of the distribution be specified. For example, if a **LOGNormal** distribution is selected for the **POrosity**, the minimum and maximum values, the mean and the standard deviation are required, as shown in Figure 4.17. The requirements for the different distributions are discussed in Section 9 of the MULTIMED model theory documentation (Salhotra et al., 1990).

Eventually, you will wish to exit the preprocessor. If you do not wish to save any of the changes you have made to the input file, you may simply type <Ctrl-C> at any point and the program will be terminated. However, if you would like to save your changes you will need to exit the program in the following manner:

1. Select the **Return** option from the screen menus until you return to the **Edit (BE)** screen.

2. Select the **Return** (to **Build** screen) option from the **Edit** screen.

3. If undefined parameters exist, the Return (BER) screen will be displayed as shown in Figure 4.18. This screen lists the data groups which contain undefined parameters. At this point, you may either 1) Return to the **Edit** screen and specify the remaining undefined parameters or 2) Return to the **Build** screen and ignore these undefined parameters.

4. From the **Build/Modify** screen (Figure 4.2), select the **Save** option by typing <S>.

5. The **Save (BS)** screen will now be displayed as shown in Figure 4.19. The name of the input file for use in MULTIMED should be specified on this screen. Note that you should use a name which is compatible with your computer system. For example, the DOS operating system on an IBM PC will allow at most 8 characters in the main filename and 3 characters in the extension on the filename. Other operating systems may have different restrictions. Press <F2> to return to the **Build/Modify** screen.

6. To exit the program, select the **Return** (to **Opening screen**) option from the **Build/Modify** screen by typing <R>.

7. The execution of MULTIMED must be done from the operating system of your computer. Therefore, select the **Return** (to operating system) option from the **Opening screen.**

4.1.2 The PREMED Tutorials

Two tutorials are included with the preprocessor. These tutorials are intended to familiarize a user with the options and utilization of PREMED. It is strongly recommended that an inexperienced user take advantage of the tutorials provided with MULTIMED. Completion of these tutorials creates complete input files for use in MULTIMED.

The tutorials are specific to the application of MULTIMED to Subtitle D facilities. One tutorial generates an input file for deterministic, steady-state simulation of flow and transport in the unsaturated zone, and transport in the saturated zone. The second tutorial is similar to the first tutorial except that it is run in a Monte Carlo framework. The input generated by the Deterministic tutorial, and the corresponding MULTIMED output, are discussed in Section 7.2. Input and output for the Monte Carlo tutorial are presented in Section 7.3.

To utilize either of these tutorials, you must first begin the preprocessor program by typing <PREMED> (do not type the brackets) from the DOS operating system. After a few seconds, the **Opening screen** for the preprocessor will appear. To activate the tutorials you must type either <@DETER.LOG> for the Deterministic tutorial, or <@MONTE.LOG> for the Monte Carlo tutorial.

The tutorial will be presented in a small box on the right hand side of the screen. An example of a tutorial screen is shown in Figure 4.20. Directions for completing the tutorial will appear in this box. In the tutorial, you will edit a pre-existing input file which is almost complete. This input file has been specially designed to contain a small number of parameters which still need values. These are called "undefined" parameters, and will need to be supplied to the preprocessor in order to complete the input file. The tutorial will provide instructions so that you can complete the file. In the process, many of the options in the preprocessor will be demonstrated.

Successful completion of the tutorials will generate the completed input sequence shown in Tables 7-4 and 7-7. These input sequences can then be used to run MULTIMED and generate the output in Tables 7-5 and 7-8. Output from the Monte Carlo tutorial, can be used with the postprocessor, POSTMED.

4.2 - THE POSTPROCESSOR (POSTMED)

The postprocessor can be used to generate plots to show the results of Monte Carlo analyses or concentration versus time. These plots are generated from the main output file and "SAT1.OUT" which are generated by MULTIMED during execution. For comparison of different simulations, POSTMED allows up to three different data files to be plotted on the same graph. Output from POSTMED may be written to the screen, to a printer, to a plotter, or to a file in text form.

4.2.1 Use of the Postprocessor

Before using the postprocessor, read the section on installation and execution of MULTIMED (Section 2).

In order to use POSTMED, you must copy the appropriate MULTIMED output file into the directory which contains the postprocessor. For Monte Carlo Analyses, the MULTIMED output file "SAT1.OUT" is used, which is generated automatically during execution of MULTIMED. Note that the "SAT1.OUT" file will be overwritten each time the model is run. Therefore, if you wish to save this file for use with the postprocessor, you should rename it. This is particularly important if you want to plot the results from more than one simulation on the same graph; the "SAT1.OUT" files for each simulation must be given a different name. For Concentration versus Time plots, the file which should be copied into the POSTMED directory is the main output file. POSTMED will select the information necessary for generating Concentration versus Time plots from this file.

To execute the postprocessor, move to the directory which contains the postprocessor and type <POSTMED> (do not type the brackets). After a moment the **Opening screen** will appear, as shown in Figure 4.21. Use the **Data** option of the **Opening screen** to provide the postprocessor with information about MULTIMED data files which you wish to plot. Type a <D> (do not type the brackets) to select this option.

POSTMED will now display the **Data-1 (D)** screen. The number of Multimedia Model runs which you wish to plot should be entered on this screen. The valid values which may be entered on this screen can be seen by pressing the <F5> key. The limits for the parameter will then be displayed in the center, assistance window, as shown in Figure 4.22. As you can see, a minimum of 1 and a maximum of 3 runs may be plotted on a single graph.

After entering a value on **Data-1 (D)** screen, select the "Next" option by pressing <F2> to go to the next screen. The **Data-2 (D)** screen will now be displayed (Figure 4.23). This screen is used to enter the name of the file(s) which contain MULTIMED results to be plotted. This screen will appear once for each run. After entering the name of the file, press <F2> to go to the next screen.

After entering the last file, the postprocessor returns to the **Opening screen.** Type <S> to describe the specifications of the plot. POSTMED will now display the **Specs (S)** screen as shown in Figure 4.24. Several options are available on this screen.

1. The Graphics device must be specified. You may send the plot generated by POSTMED to the screen (DISPLAY), a printer or a plotter. If your computer will not support graphics, it may be desirable to send the plot directly to a printer. Alternatively, the coordinates used to generate the plot may be sent either to the screen or to a TEXT file.

2. The X- and Y-axis types must be specified. Either arithmetic or logarithmic scales may be used. Note that logarithmic scales can not be used with FREQUENCY plots. If a logarithmic scale is selected, the number of logarithmic cycles for each axis must be specified.

3. The location of the legend on the plot must be specified. The options are: UL (upper left), LL (lower left) , UR (upper right), LR (lower left).

4. You must specify the type of plot you wish to create. Three choices are allowed: a cumulative frequency plot (CUMULATIVE), a frequency plot (FREQUENCY) or a concentration versus time plot (TIME). The FREQUENCY plot provides information about the number of times a particular concentration was obtained, which is displayed in histogram format. Selection of the CUMULATIVE option will generate a plot showing the cumulative frequency of concentration values. The TIME option plots concentration versus time for <u>transient</u> runs.

5. The Y minimum and Y maximum (in percent) of the plot should be specified. The minimum value must be less than the maximum.

To move between options, press <carriage return>. To select an option, type enough characters to make the selection unique. For example, the Graphics device options (Figure 4.24) are: DISPLAY, PRINTER, PLOTTER, TEXT, SCREEN. If you wish to select DISPLAY, you may type only <D>. However, if you want to send your results to a printer, you must type two characters, <PR>, since there are two options beginning with "P". Once you have selected the desired options on the **Specs (S)** screen, press <F2> to return to the **Opening screen.**

Titles for the Graph, the x- and y-axis, and the different runs can be entered on the **Titles (T)** screen. From the **Opening screen,** type <T> for this selection. This screen is shown in Figure 4.25. Any character string may be used as a title. Use the <carriage return> to move between options. Press <F2> to return to the **Opening screen.**

Now you are ready to generate a plot. If you wish to make any changes to the any of the screens, type the first letter of the menu item to select the option, make the necessary changes, and return to the **Opening screen** by pressing <F2>. Otherwise, type <P> to generate the plot. The plot will then be sent to the Graphics device that you specified on the **Specs (S)** screen. A cumulative frequency plot showing the results of the simulation of an example problem is presented in Figure 4.26. The corresponding frequency plot is shown in Figure 4.27. Figure 4.28 shows the first screen of the text file generated by selecting the SCREEN option for the same example problem. Selection of the TEXT option will send the same file to a specified file.

Now, you may either repeat the process described above and generate additional plots, or type <R> to return to the operating system.

Figure 4.26

Figure 4.27

SECTION 5

MODEL APPLICATION

The large number of interrelated physical, chemical and biological processes involved in the migration of leachates from waste disposal facilities makes the prediction of groundwater contamination from these facilities a complex task. Mathematical models are useful tools which provide insight into the effects on groundwater quality of facility design, operation and failure.

All models are simplified representations of the real system; no model will ever reproduce the exact characteristics of a site. Therefore, model results should always be interpreted as estimates of groundwater flow and contaminant transport, and not as exact predictions. Bond and Hwang (1988) recommend that models be used for comparing various cases or scenarios, since all cases are subject to the same limitations and simplifications. Furthermore, models are useful for sensitivity analysis, determining the effects of varying one parameter on the model results. It is important to understand the limitations of mathematical models, and to use them correctly in evaluation of actual environmental conditions.

Several recent reports present detailed discussions of the issues related to model selection, application, and validation. Donigian and Rao (1988) address each of these issues. Issues related to model selection and application are addressed in detail by Boutwell et al. (1986). Weaver et al. (1989) discuss the selection and field validation of mathematical models. In addition, a report by the National Research Council (1990) discusses model application and validation and provides recommendations for the proper use of groundwater models. Model users, particularly those who are relatively inexperienced, are encouraged to read these and similar reports before beginning a modeling study.

The validity of the results from mathematical models depends to a large extent on the proper application of the model. The application of a model to a leachate migration problem requires several steps. First, the modeling needs and the objectives of the study should be determined. Next, data should be collected for characterization of the hydrological, geological, chemical and biological conditions present in the system. These data should assist in the development of the "scenario" to be modeled, which provides the framework for the conceptual model of the system. The conceptual model and data are used to verify that the selected model is appropriate. During model application, results should be calibrated to obtain the best fit to observed data. Finally, these results should be validated by comparing them to independently-derived data or observations.

In order to apply a model to a specific site, it is necessary to describe the "scenario" to be represented by the model. A scenario is essentially a description of all the important processes and characteristics of a particular site. Although it may be possible to describe the "average" characteristics of a Subtitle D landfill or surface impoundment, it would be dangerous to assume that this description adequately describes all such facilities. Each site is unique, and must be characterized separately. This section describes some of the issues which should be considered when developing a scenario and using MULTIMED to represent the conceptual model of the site.

One of the most severe limitations to modeling is insufficient data. Uncertainty in model predictions results from our inability to characterize a site in terms of the boundary conditions or the key parameters describing the important flow and transport processes (National Research Council, 1990). The results of MULTIMED are highly dependent on the quantity and quality of the available data. The application of MULTIMED to a site requires the collection of a large amount of data, and the process of applying MULTIMED to a scenario may reveal data deficiencies which require additional data collection.

Based on the available data and the judgement of the modeler, values of the required parameters should be determined. Parameter values which must be determined for Subtitle D applications are discussed in Section 5.3. Section 6 of this manual provides guidance for estimation of parameters for use in MULTIMED. Inexperienced modelers may attempt to apply the model when the lack of site-specific data causes the model results to be highly speculative. It must be emphasized that a mathematical model should never be used as a substitute for data in site-specific applications.

As stated above, the conceptual model and data should be used to determine whether or not a mathematical model is appropriate for representing the subsurface system and which options in the model should be utilized. The model should:

- Allow the objectives of the study to be achieved
- Adequately simulate the significant processes present in the actual system
- Be consistent with the complexity of the study area
- Be appropriate for the amount of available data

Some of the factors which should be considered before applying MULTIMED to a particular site are summarized in Table 5-1. This list is not exhaustive, and is meant only to provide guidance. The factors in Table 5-1 are addressed in terms of MULTIMED's capabilities and limitations in the following section.

5.1 MULTIMED CAPABILITIES AND LIMITATIONS

5.1.1 Solution Techniques

MULTIMED utilizes analytical and semi-analytical solution techniques to solve the mathematical equations describing flow and transport. These solution

TABLE 5-1. ISSUES TO BE CONSIDERED BEFORE APPLYING MULTIMED

Objectives of the Study

- Is a "screening level" approach appropriate?
- Is modeling a "worst-case scenario" acceptable?

Significant Processes Affecting Contaminant Transport

- Does MULTIMED simulate all the significant processes occurring at the site?
- Is the contaminant soluble in water and of the same density as water?

Accuracy and Availability of the Data

- Have sufficient data been collected to obtain reliable results?
- What is the level of uncertainty associated with the data?
- Would a Monte Carlo simulation be useful? If so, are the cumulative probability distributions for the parameters with uncertain values known?

Complexity of the Hydrogeologic System

- Are the hydrogeologic properties of the system uniform?
- Is the flow in the aquifer uniform and steady?
- Is the site geometry regular?
- Does the source boundary condition require a transient or steady-state solution?

techniques have advantages and disadvantages over fully numerical models. Analytical solutions are computationally more efficient than numerical simulations and are more conducive to uncertainty analysis (i.e. Monte Carlo techniques). Typically, input data for analytical models are simple and they do not require detailed familiarity with the code or extensive modeling experience. Analytical solutions are typically the most efficient alternative when data necessary for the characterization of the system are sparse (Javandel et al., 1984). The limited data available in most field situations may not justify the use of a detailed numerical model; in some cases, results from simple analytical models may be just as meaningful (Huyakorn et al., 1986).

However, analytical models require simplifying assumptions about the system which are not necessary for numerical models. These simplifications result in models which include relatively few processes and a limited number of parameters which are often required to be constant in space and time (van der Heijde and Beljin, 1988). MULTIMED is no exception; the representation of the system simulated by the model is simple, and little or no spatial or temporal variability is allowed for the parameters in the system.

Bond and Hwang (1988) present guidelines for determining whether the assumption of uniform aquifer properties is justified at a particular site. In more complex systems, it may be beneficial to use MULTIMED as a "screening level" model which would allow a user to obtain an understanding of the system. A numerical model could then be used if there are sufficient data and necessity to justify the use of a more complex model.

A highly complex hydrogeological system cannot be accurately represented with MULTIMED. Heterogeneous or anisotropic aquifer properties, multiple aquifers and complicated boundary conditions cannot be simulated using this model. MULTIMED cannot simulate processes, such as flow in fractures and chemical reactions between contaminants, which can have a significant effect on the concentration of contaminants at a site. Since each site is unique, it must be left to the modeler to determine which conditions and processes are important at a specific site, and to determine the suitability of applying MULTIMED.

5.1.2 Spatial Characteristics of the System

Although actual landfills and groundwater systems are three-dimensional, it is common to reduce the number of dimensions simulated in a mathematical model to one or two. Two and three-dimensional models are generally more complex and computationally expensive than one-dimensional models, and therefore require more data. In some instances, a one-dimensional model may adequately represent the system. Furthermore, the available data may not warrant the use of a multidimensional model.

However, modeling a truly three-dimensional system using a one-dimensional model may produce inaccurate results. Three-dimensional effects are often very significant in describing processes such as contaminant plume migration. The choice of the number of dimensions in the model should be made for a specific site, based on the conditions present at that site. The information which is desired from the model output should also be considered.

MULTIMED has the following spatial characteristics:

- The Unsaturated Flow Module simulates vertical, one-dimensional flow.
- The Unsaturated Transport Module simulates vertical, one-dimensional transport. Dispersion is only considered in the longitudinal (vertical) direction.

- The Saturated Transport Module assumes one-dimensional, horizontal flow. However, three-dimensional dispersion may be simulated since the effects of lateral or vertical dispersion may significantly affect the model results.

These spatial assumptions should be considered when applying MULTIMED to a site. The assumption of flow only in the vertical direction may be valid for facilities which receive uniform areal recharge. The assumption may not be valid in facilities where surface soils (covers or daily backfill) or surface slopes result in an increase of runoff in certain areas of the facility and ponding of precipitation in others (Kirkham et al., 1986).

The simulation of one-dimensional, horizontal flow in the saturated zone requires several assumptions. The saturated zone is treated as a single, horizontal aquifer with uniform properties. The effects of pumping or discharging wells on the groundwater flow system cannot be considered. These assumptions should be considered when applying MULTIMED to a site.

5.1.3 Steady-State versus Transient Flow and Transport

The MULTIMED model assumes steady-state flow in all applications. Some groundwater flow systems are in an approximate "steady-state", in which the water entering the flow system is balanced by the water leaving the system. There is no significant temporal variation in the system. The assumption of steady-state conditions in a model generally simplifies the mathematical equations used to describe processes, and reduces the amount of input data, since no information about temporal variability is necessary.

However, assuming steady-state conditions in a system which exhibits transient behavior may produce inaccurate results. For example, climatic variables, such as precipitation vary in time and may have strong seasonal components. In such areas, the assumption of constant recharge of the groundwater system is incorrect. In general, this assumption will cause underestimation of contaminant concentrations in the subsurface, since steady-state models can not simulate the effects of individual storms, which can provide a substantial driving force for contaminant transport.

MULTIMED can simulate either steady-state or transient transport conditions. The assumption of steady-state transport requires that the contaminant source has a sufficiently large mass to ensure that the downgradient concentration, once reached, will be maintained (Mulkey et al., 1989). It must be assumed that the source is continuous and constant. If these assumptions can not be made at a particular site, inaccurate results will be produced by a steady-state transport model. Steady-state models are also inappropriate when the simulation includes chemicals which sorb or transform significantly (Mulkey et al., 1989). Note that although the steady-state model can be very conservative, this may be appropriate for some applications. The choice of simulating steady-state or transient conditions should be made based the objectives of the study and on the degree of temporal variability in the system.

5.1.4 Monte Carlo versus Deterministic Simulations

MULTIMED may be run in either a deterministic or a Monte Carlo framework. In a deterministic simulation, exactly one model result is determined for a given set of input values. All of the input variables are assumed to have a fixed mathematical relationship with each other, which completely define the system. Monte Carlo simulations, however, consider the intrinsic randomness and uncertainties inherent in the system. The Monte Carlo method provides a means of estimating the uncertainty in the results of a model, if the uncertainty of the input variables is known or can be estimated. For each of the uncertain variables, a cumulative probability distribution must be determined. The Monte-Carlo technique involves running a model a large number of times with different values of input parameters, which are determined from probability distributions, and then analyzing the results. The Monte Carlo option is discussed in Section 9 of the MULTIMED model theory documentation (Salhotra et al., 1990).

There are many sources of uncertainty in the prediction of leachate migration in the subsurface. Uncertainties may be due to measurement error in parameters which describe the physical and chemical properties of the system, the presence of spatial and temporal variability in the parameters, or incompletely understood processes which are simulated by the mathematical model. There may be some uncertainty associated with extrapolating data from one set of conditions to a different set of conditions. Therefore, it may be more appropriate to express these uncertain input parameters in terms of a probability distribution rather than a single deterministic value and to use an uncertainty propagation model to assess the effect of the variability on the model output (Salhotra and Mineart, 1988).

The specified uncertainty in the input parameters for MULTIMED is highly site-specific. Available data for many sites are scarce and even sites which are very well-characterized may exhibit a substantial amount of variability in measured parameter values. Most of the parameters in the MULTIMED model may be assigned a Monte Carlo distribution. It must be left to the user of the MULTIMED model to determine which input parameter values are uncertain at a particular site.

Although the Monte-Carlo method can be a useful tool for quantitatively evaluating uncertainty in a model, it is not without problems. One difficulty is related to determining the cumulative probability distribution for a given parameter. These distributions must be determined from a large amount of data, which may not be available. Assuming a parameter probability distribution when the distribution is unknown does not help reduce uncertainty, as the certainty of the output is then a function of the assumed certainty of the input parameter (U.S. EPA, 1988). Furthermore, in order to obtain a valid estimate of the uncertainty in the output, the model must be run numerous times (typically at least several hundred times) which can be computationally expensive. These issues should be considered before utilizing the Monte-Carlo technique.

5.1.5 Boundary conditions

The source boundary condition for MULTIMED relates to the introduction of the contaminant to the aquifer system. MULTIMED is limited to relatively simple representations of the source of groundwater contamination. Only two types of source geometries can be simulated by MULTIMED: a patch source or Gaussian distributed source. Temporally, these source geometries may be described as either: 1) continuous 2) exponentially decaying or 3) a non-decaying pulse of finite duration. These types of sources are discussed in Section 5 of the MULTIMED model theory documentation (Salhotra et al., 1990).

5.2 SUBTITLE D APPLICATIONS OF MULTIMED

5.2.1 Summary of EPA Requirements for MULTIMED Simulations of Leachate Migration from Subtitle D Facilities

The U.S. EPA has developed several restrictions for Subtitle D applications of MULTIMED. These restrictions were made in an effort to develop a conservative approach for simulating leachate migration from Subtitle D facilities.

- Only the Saturated and/or Unsaturated Modules may be active in Subtitle D applications, because the Surface Water, Landfill and Air Modules have not been sufficiently tested at this time.

- Although MULTIMED can simulate either steady-state or transient transport conditions, only steady-state transport simulations are allowed for Subtitle D applications. No decay of the source term is allowed; the concentration of contaminants entering the aquifer system must be constant in time. The contaminant pulse is assumed continuous and constant for the duration of the simulation.

- The receptor must be located directly downgradient of the facility, so that it intercepts the center of the contaminant plume. In addition, the contaminant concentration must be calculated at the top of aquifer. Therefore, the angle from the plume centerline to the receptor and the vertical distance to the receptor must be specified as zero in Subtitle D applications.

- Only the Gaussian source geometry is allowed in Subtitle D applications.

The application of MULTIMED to Subtitle D facilities simulates the transport of contaminants from the source, through the saturated and/or unsaturated zones by groundwater, and to a receptor (i.e. a well). Although the Landfill Module in MULTIMED can not be used at present because it has not been sufficiently tested, MULTIMED can be used in conjunction with another source model, such as HELP (Schroeder et al., 1984), to develop and compare the effects of different facility designs on groundwater quality. MULTIMED combined with a source model could be used to demonstrate that either the landfill design, or the specific hydrogeologic conditions present at the site will prevent the migration of significant quantities of leachate from the landfill. Furthermore, MULTIMED could be used to predict the results of different types of "failure" of the landfill. If leachate migration into the groundwater below a waste disposal facility occurs, MULTIMED could be useful in predicting the fate and transport of the contaminants in the subsurface.

5.2.2 Active Modules

Flow and transport in the subsurface typically occurs through the unsaturated zone, to the water table and into the saturated zone. However, in some instances, the water table may be located just below the waste disposal facility, so that only saturated flow and transport away from the facility need to be considered. Therefore, two basic simulation options are allowed for Subtitle D applications of MULTIMED: 1) flow and transport in the unsaturated zone coupled with transport in the saturated zone or 2) saturated transport only. The simulation of the system should accurately represent the

moisture conditions present at the site.

Simulation of these options in MULTIMED requires that the Saturated Zone Module, and, if the water table is located at a significant depth below the waste disposal facility, the Unsaturated Flow and Transport Modules, be active. Use of the Saturated Zone Module requires four data groups: the General, Chemical, Source, and Saturated Zone Data Groups. If the Unsaturated Flow and Transport Modules are active, two additional data groups must be used: the Unsaturated Flow and Transport Data Groups. The parameters required in each of these data groups are discussed in Section 5.3.2.

5.2.3 Boundary conditions

Although MULTIMED can simulate two source geometries, only the Gaussian distributed source is allowed in Subtitle D applications. Temporal variation in the source term boundary conditions in MULTIMED are not allowed for Subtitle D applications, which must be run in steady-state. Therefore, although constant pulse and exponential decay boundary conditions are allowed for generic applications of MULTIMED, only a constant source is allowed in Subtitle D applications.

5.2.4 Procedure for Application of MULTIMED to Subtitle D Facility Design

MULTIMED can be used to assist in the design of Subtitle D landfills (Figure 5.1). As the flowchart shows, the role of MULTIMED in the design process is to evaluate the ability of a particular design to insure that groundwater concentrations of chemicals expected to exist in Subtitle D landfills do not exceed health based thresholds. A step-wise procedure for determining the minimum design necessary to protect groundwater at these levels and keyed to the flowchart shown in Figure 5.1 follows:

1) Collect site-specific hydrogeological data. These data may include aquifer particle size, porosity, bulk density, hydraulic conductivity and gradient, groundwater velocity, dispersivities, and thickness.

Figure 5.1

Lists and a discussion of the parameters required for Subtitle D applications of MULTIMED are presented in Section 5.3. See Section 6 for guidance in parameter estimation.

2) Based on water level measurements, determine whether or not the Unsaturated Zone Modules should be active in the simulation. If the unsaturated zone will be simulated, collect site-specific data on the properties of the unsaturated zone.

3) Determine contaminant which will be simulated. The selection of the contaminant to be simulated may be based on a variety of factors or it may be prescribed. It may be a chemical which is particularly persistent in the subsurface environment, or is present in high concentrations in the specific Subtitle D facility. Determine chemical properties for the selected contaminant (see Section 6).

4) Propose landfill design and determine the infiltration rate at the site. This can be done using a water balance model, such as HELP (Schroeder et al., 1984), which includes representations of engineering controls. Note that infiltration rate as used here means the volumetric flow rate in meters per year from the bottom of the landfill into the unsaturated zone or aquifer. Obviously, the attenuation of this flow is the objective of landfill engineering controls. For each specific landfill design, there is a resulting steady-state infiltration rate.

5) Run MULTIMED using the Subtitle D application type, the hydrogeological data collected in Step 1, the infiltration rate determined in Step 2, and with the point of compliance set to the required location. As discussed above, the Subtitle D application assumes steady-state conditions and the point of compliance (POC) must be along the plume centerline. You may wish to set the input leachate concentration to 1.0 mg/l for convenience in later calculations (see step 6).

6) The EPA-recommended criteria for establishing whether or not a particular design is acceptable is based on the dilution-attenuation factor (DAF). This method is based on the fact that the model estimate of concentration at the point of compliance is linear with respect to the input concentration. Therefore, the DAF is the factor by which the concentration is expected to decrease between the landfill and the point of compliance.

Using the concentration predicted by MULTIMED at the point of compliance, the dilution-attenuation factor (DAF) for the landfill/aquifer system may be calculated using the following equation:

DAF = leachate concentration / concentration at the POC

or, if the leachate concentration is 1.0 mg/l in the model,

DAF = 1.0 / concentration at the POC

7) If the DAF is equal to or greater than 100, the design is acceptable (see discussion below). Otherwise, the landfill design must be made more stringent by increasing the number or effectiveness of engineering controls so that the infiltration rate is reduced. To evaluate the new design, repeat Steps 2-5. Continue until an acceptable design is reached (DAF is equal to or greater than 100).

The threshold DAF of 100 is used to define an acceptable design because the maximum allowable leachate concentration of chemicals expected to exist in a Subtitle D landfill is 100 times the Maximum Contaminant Level (MCL) for each chemical (U.S. EPA, 1990). This approach to determining the expected concentration of constituents in leachate from a Subtitle D landfill is attractive because of its consistency with other regulations and its generic nature. If site-specific conditions permit the use of other approaches which are acceptable to an approved state, these may be used.

5.3 MULTIMED INPUT REQUIREMENTS

As discussed above, the MULTIMED code consists of seven modules which are described in Salhotra et al. (1990). Only three of the modules can be used for Subtitle D applications of the model: the Saturated Zone Transport Module, the Unsaturated Zone Flow Module, and the Unsaturated Zone Transport Module. The Saturated Zone Transport Module is required for all Subtitle D applications and can be applied independently of the Unsaturated Zone Modules. Depending on site-specific conditions, the Unsaturated Zone Modules may or may not be needed. Note that the two Unsaturated Zone Modules must be used in conjunction with each other and with the Saturated Zone Module.

The operation of each module requires specific input, which is organized into data groups. The General Data Group, which is required for all simulations, contains flags and data which describe the scenario being modeled. The input parameters needed for the Saturated Zone Transport Module are found in three additional data groups: the Chemical Data Group, the Source Data Group, and the Aquifer Data Group. Use of the Unsaturated Zone Modules requires input found in the same data groups, as well as two others: the Unsaturated Zone Flow Data Group and the Unsaturated Zone Transport Data Group.

In this section, parameter requirements are discussed in two stages. Section 5.3.1 introduces the input parameters required by each of the three modules which can be active in Subtitle D applications. In Section 5.3.2, the parameters in each data group are presented and the options available for specifying their values in the code are summarized. Help in estimating these parameters is provided in Section 6.

5.3.1 Parameter Requirements Summarized by Module

5.3.1.1 The Saturated Zone Transport Module--

The primary input parameters required to compute a contaminant concentration in the saturated zone for Subtitle D applications are shown in Table 5-2, organized according to the data group in which they are found. A number of the parameters listed in Table 5-2 can be derived using other variables and a set of empirical, semi-empirical, or exact relationships. Note that some of the parameters used to derive the primary parameters can also be derived. Table 5-3 indicates which parameters can be derived and lists the additional variables needed. The methods used to derive the parameters are described in Section 6 of this document or in Section 5.5 of Salhotra et al. (1990). Note

that both particle diameter and porosity can not be simultaneously derived, since one is derived from the other.

5.3.1.2 The Unsaturated Zone Flow Module--

The input parameters required to compute flow in the unsaturated zone are shown in Table 5-4. Note that only one input variable in the Source Data Group is needed. The remaining variables are all located in the Unsaturated Zone Flow Data Group. None of these parameters can be derived.

5.3.1.3 The Unsaturated Zone Transport Module--

Table 5-5 lists the parameters used to compute contaminant transport in the unsaturated zone. The variables are located in five different data groups. Note that an overall chemical decay coefficient and distribution coefficient for the unsaturated zone can not be entered directly, as they can in the saturated zone module. Rather, they are calculated in the code using methods described in Section 5.5.2.1 of Salhotra et al. (1990). Of the parameters shown in Table 5-5, only the longitudinal dispersivity can be derived.

5.3.2 Parameter Requirements Summarized by Data Group

This section is written with the assumption that the modeler will use the preprocessor, PREMED, to create and modify input files for Subtitle D applications (see Section 4). Thus, the organization of the information in this section is compatible with that of the preprocessor. The parameters are listed in tables according to data group. Further, the parameters listed in each of the data group tables are organized according to the preprocessor screen in which they can be found. Advanced users, who choose to modify input files directly without the use of the preprocessor, will notice that there is some discrepancy between the organization of data in the preprocessor (and this section) and the structure of the input file, which is discussed in Appendix A.

5.3.2.1 General Data Group--

The General Data Group screens of the preprocessor contain flags which allow the user to specify the run options and active modules for the input file. The choices made in this data group determine which parameters must be specified in
the rest of the input. Therefore, the General Data Group should always be

TABLE 5-2. PRIMARY PARAMETERS USED IN THE SATURATED ZONE TRANSPORT MODULE FOR SUBTITLE D APPLICATIONS OF MULTIMED

Parameters	Units
Source Data Group Parameters	
Area of the land disposal facility	[m^2]
Leachate concentration at the waste facility	[mg/l, g/m^3]
Recharge rate into the plume	[m/yr]
Infiltration rate from the facility	[m/yr]
Standard deviation (i.e., spread) of the source	[m]
Aquifer Data Group Parameters	
Type of source geometry (only Gaussian allowed)	
Porosity	[cc/cc]
Thickness of the aquifer	[m]
Thickness of source (i.e., mixing zone depth)	[m]
Seepage velocity	[m/yr]
Dispersivities (longitudinal, transverse, vertical)	[m]
Retardation coefficient [dimensionless]	
Radial distance from the site to the receptor	[m]
Chemical Data Group Parameters	
Effective first-order decay coefficient	[1/yr]
Distribution coefficient	[cc/g]

TABLE 5-3. PARAMETERS USED TO DERIVE OTHER SATURATED ZONE TRANSPORT MODULE PARAMETERS NEEDED IN SUBTITLE D APPLICATIONS OF MULTIMED

Parameters	Units
Overall Chemical Decay Coefficient	
Biodegradation rate	[1/yr]
Solid phase decay coefficient	[1/yr]
Dissolved phase decay coefficient	[1/yr]
Bulk density	[g/cc]
Distribution coefficient	[cc/g]
Porosity	[cc/cc]
Solid and Dissolved Phase Decay Coefficients	
Reference temperature	[°C]
Aquifer temperature	[°C]
Second-order acid-catalysis hydrolysis rate constant at reference temperature	[ℓ/mole-yr]
Second-order base-catalysis hydrolysis rate constant at reference temperature	[ℓ/mole-yr]
Neutral hydrolysis rate constant at reference temperature	[1/yr]
pH of the aquifer	[pH units]
Retardation Coefficient	
Bulk density	[g/cc]
Distribution coefficient	[cc/g]
Porosity	[cc/cc]
Bulk Density	
Porosity	[cc/cc]
Porosity	
Mean particle diameter of the porous medium	[cm]
Particle Diameter	
Porosity	[cc/cc]

(continued)

TABLE 5-3. PARAMETERS USED TO DERIVE OTHER SATURATED ZONE TRANSPORT MODULE PARAMETERS NEEDED IN SUBTITLE D APPLICATIONS OF MULTIMED (concluded)

Parameters	Units
Distribution Coefficient	
Normalized distribution coefficient for organic carbon, K_{oc}	[cc/g]
Fractional organic carbon content	[dimensionless]
Seepage Velocity	
Hydraulic gradient	[m/m]
Hydraulic conductivity	[m/yr]
Porosity	[cc/cc]
Hydraulic Conductivity	
Porosity	[cc/cc]
Mean particle diameter of the porous medium	[cm]
Thickness of the Source (Mixing Zone Depth)	
Length of the land disposal facility	[m]
Thickness of the aquifer	[m]
Seepage velocity	[m/yr]
Porosity	[cc/cc]
Infiltration rate through the facility	[m/yr]
Vertical dispersivity	[m]
Standard Deviation of the Source	
Width of the land disposal facility	[m]
Length and Width of the Facility	
Area of the land disposal facility	[m^2]
Dispersivities	
Radial distance from the site to the receptor	[m]

TABLE 5-4. PARAMETERS REQUIRED IN THE UNSATURATED ZONE FLOW MODULE FOR SUBTITLE D APPLICATIONS OF MULTIMED

Parameter	Units
Source Data Group Parameters	
Infiltration rate from the facility	[m/yr]
Unsaturated Zone Data Group Parameters	
Number of physical flow layers	[dimensionless]
Number of porous materials	[dimensionless]
Thickness of each layer	[m]
Material associated with each layer	[dimensionless]
For each material:	
Air entry pressure head	[m]
Porosity	[dimensionless]
Saturated hydraulic conductivity	[cm/hr]
Residual saturation (water content)	[dimensionless]
Either:	
van Genuchten alpha coefficient	[1/cm]
van Genuchten beta coefficient	[dimensionless]
or	
Brooks and Corey exponent	[dimensionless]
van Genuchten alpha coefficient	[1/cm]
van Genuchten beta coefficient	[dimensionless]

Note: The model provides the option to use either van Genuchten's or Brooks and Corey's constitutive relationship for relative permeability versus water saturation. However, the relationship between pressure head and water saturation is expressed in terms of van Genuchten parameters.

TABLE 5-5. PARAMETERS REQUIRED IN THE UNSATURATED ZONE TRANSPORT MODULE FOR SUBTITLE D APPLICATIONS OF MULTIMED

Parameters	Units
Source Data Group Parameters	
Source concentration at top of unsaturated zone	[mg/ℓ]
Unsaturated Zone Transport Data Group Parameters	
Control parameters related to the evaluation schemes used in the module	
Number of layers used to simulate transport	[dimensionless]
For each layer:	
Thickness	[m]
Longitudinal dispersivity	[m]
Bulk density of the soil	[g/cc]
Biodegradation rate,	[1/yr]
Percent organic matter	[dimensionless]
Unsaturated Zone Flow Data Group Parameters	
Porosity of the unsaturated zone	[cc/cc]
Aquifer Data Group Parameters	
Temperature of the aquifer[a]	[°C]
pH of the aquifer[a]	[pH units]
Chemical Data Group Parameters	
Normalized distribution coefficient (i.e., K_{oc})	[cc/g]
Reference Temperature	[°C]
Acid and base hydrolysis rates at reference temperature	[ℓ/mole-yr]
Neutral hydrolysis rate at reference temperature	[1/yr]

[a] Note: the temperature and pH used in calculating the unsaturated zone overall chemical decay rate are the temperature and pH specified for the aquifer.

completed first. The information which needs to be supplied for all model applications is:

Title--Two lines of text can be entered. The text, which is used to label the input and output, can consist of two character strings, each up to 78 characters in length.

Run Option--The default run option is **Deterministic**. However, the user has the option of selecting a Monte Carlo run instead. Issues related to the choice between these two options are addressed in Section 5.1.4. In addition, Monte Carlo simulations are discussed in Section 9 of Salhotra et al. (1990).

Active Modules--For Subtitle D applications, the default for active modules is **Unsaturated Zone/Saturated Zone**. However, the user can choose that the Saturated Zone alone be active. The Air, Landfill, and Surface Water Modules can not be accessed for Subtitle D applications.

Transient versus Steady-state--For Subtitle D applications, the user has no choice for this flag. Simulations must be steady-state.

For Monte Carlo simulations, additional information is required in the General Data Group. The additional information is:

Number of Monte Carlo Simulations--Typically hundreds to thousands of Monte Carlo simulations are needed to obtain meaningful results. Section 9.9 of Salhotra et al. (1990) provides information on the estimation of this value.

Level of Output from Monte Carlo Runs--The default for this flag is **SOME**, which means that the main output file and the STATS.OUT and SAT1.OUT files are created (see Section A.2 for a description and listing of the output files). The two other options available to the user are LOTS, which opens the maximum number of output files, and NONE, which opens only the main and STATS.OUT files. Note that in order to use the postprocessor to create frequency and cumulative frequency plots, the file SAT1.OUT is needed and thus, this flag must be set to either LOTS or SOME. A few of the files created using the LOTS flag can be very large, depending on the number of Monte Carlo simulations. On many PC computers, these files can fill all available disk space and cause the simulation to fail. Thus, on PC's the default of **SOME** is recommended.

Confidence Level (in percent) for the Four Estimated Percentiles--In Monte Carlo mode, MULTIMED calculates confidence bounds for the 80th, 85th, 90th, and 95th percentiles. The confidence bounds are discussed in Section 9.8 of Salhotra et al. (1990).

5.3.2.2 Chemical Data Group--

The MULTIMED parameters contained in the Chemical Data Group are shown in Table 5-6. Note that some of the parameters are associated with the Surface Water and Air Modules of MULTIMED and thus, are not used for Subtitle D applications of the model. Further, note that five of the parameters (i.e., the solid phase, liquid phase, and overall decay coefficients, the distribution coefficient, and the biodegradation coefficient) are used only in the Saturated Zone Module. Other parameters may be used by more than one model module.

TABLE 5-6. PARAMETERS IN THE CHEMICAL (Chemical) DATA GROUP

Parameter [units]	Derived				Specified					Default Value	Comments
	C	N	Ln	Exp	U	Log10U	Emp	SB	G		
Decay Coefficients:											
Solid phase decay coeff. (sat. zone) [1/yr]	–	–	–	–	–	–	–	–	–		
Dissolved phase decay (sat. zone) [1/yr]	–	–	–	–	–	–	–	–	–		
Overall chemical decay (sat. zone) [1/yr]	–	–	–	–	–	–	–	–	–		
Hydrolysis Rate Constants and Reference Temperature:											
Acid catalyzed hydrolysis [1/M-yr]	–	–	–	–	–	–	–	–		0	
Neutral catalyzed hydrolysis [1/yr]	–	–	–	–	–	–	–	–		0	
Base catalyzed hydrolysis [1/M-yr]	–	–	–	–	–	–	–	–		0	
Reference temperature [oC]	–	–	–	–	–	–	–	–			
Various Coefficients:											
Normalized distribution coeff. [ml/g]	–	–	–	–	–	–	–	–			
Distribution coeff. (sat. zone) [ml/g]	–	–	–	–	–	–	–	–	–		

C = Constant; N = Normal; Ln = Lognormal; Exp = Exponential; U = Uniform; Log10u = Log10Uniform; Emp = Empirical; SB = Johnson SB; G = Gelhar

TABLE 5-6. PARAMETERS IN THE CHEMICAL (Chemical) DATA GROUP (concluded)

Parameter [units]	Derived			Specified						Default	Comments
	C	N	Ln	Exp	U	Log10U	Emp	SB	G	Value	
Biodegradation coeff. (sat. zone) [1/yr]	–	–	–	–	–	–	–	–			

Air diffusion coeff.
Not used in Subtitle D
[cm2/s] applications.

Temperature for air
Not used in Subtitle D
diffusion [oC] applications.

Molecular Definitions, Solute Vapor Pressure, Henry's Constant:

Molecular weight [g/mole] Not used in Subtitle D applications.

Mole fraction of solute [--] Not used in Subtitle D applications.

Solute vapor pressure [mm Hg] Not used in Subtitle D applications.

Henry's Law const. [atm-m3/M] Not used in Subtitle D applications.

C	=	Constant	Exp	=	Exponential	Emp	=	Empirical
N	=	Normal	U	=	Uniform	SB	=	Johnson SB
Ln	=	Lognormal	Log10u	=	Log10Uniform	G	=	Gelhar

Table 5-6 indicates that four of the parameters in the Chemical Data Group can be derived. If the user chooses to have the code calculate the values of these parameters, additional parameters are needed (see Table 5-3). All of the Chemical Data Group parameters can be assigned a constant value or, in Monte Carlo mode, can be assigned one of seven Monte Carlo distributions. If a Monte Carlo distribution is selected for any of the parameters, additional information defining the distribution must be entered for that parameter (see Table 5-7). The Monte Carlo distributions are described in Section 9.5 of Salhotra et al. (1990). Also, limited help in determining the appropriate Monte Carlo distribution for a particular parameter is provided in Section 6.

Most of the parameters are undefined initially in the preprocessor and must have a value assigned to them before an input file can be completed. Note that three of the parameters have a default value of **zero** assigned initially. The default values can be changed at the user's discretion.

5.3.2.3 Source Data Group--

Table 5-8 lists the parameters in the Source Data Group. Note that in Subtitle D applications the source is assumed to be continuous and non-decaying. Therefore, two of the parameters, the duration of the pulse and the source decay constant, can not be modified by the user. Refer to Tables 5-2 through 5-5 in order to determine which of the remaining parameters are needed for specific model applications.

The values specified for the infiltration rate and the initial chemical concentration entering the subsurface from the facility are difficult to determine and yet are critical to the modeling effort. Refer to Section 5.2.4 for information about the values to use for these parameters when designing Subtitle D facilities. Some general information is also provided in Section 6.

Three of the parameters listed in Table 5-8 can be derived. The derivation of these parameters is described in Section 6 and Table 5-3 summarizes the parameters needed for the derivations. All of the Source Data Group parameters can be assigned a constant value or, in Monte Carlo mode, can be assigned one of seven Monte Carlo distributions described in Section 9.5 of Salhotra et al. (1990). Refer to Table 5-7 for a list of the additional parameters required when a Monte Carlo distribution is specified for an input parameter.

5.3.2.4 Aquifer Data Group--

The parameters in the Aquifer Data Group of the preprocessor are shown in Table 5-9. This data group contains the largest number of parameters of all the data groups, but many of them are "secondary" parameters (i.e., parameters used to derive the "primary" parameters or other "secondary" parameters). Depending on selections made by the user, some of these "secondary" parameters may not be used by the code. Refer to Tables 5-2 and 5-3 and to Section 6 in order to understand the relationships between these parameters and parameters in other data groups.

TABLE 5-7. PARAMETERS REQUIRED FOR SELECTED PROBABILITY DENSITY DISTRIBUTIONS

Distribution	Required Parameters
Normal	minimum, maximum, mean, standard deviation
Lognormal	minimum, maximum, mean, standard deviation
Exponential	minimum, maximum, mean
Uniform	minimum, maximum
Log_{10}uniform	minimum, maximum
Johnson SB	minimum, maximum, mean, standard deviation
Empirical	minimum, maximum, up to 20 pairs of data defining the probability and associated value (which describe the distribution)

The parameters used to specify well location are restricted in Subtitle D applications. Only the downgradient distance from the site can be input by the user. Otherwise, it is assumed that the well is on the plume centerline and screened at the top of the aquifer. The well angle off center and vertical distance can not be modified, nor can they be assigned a Monte Carlo distribution.

In the preprocessor, the geometry of the source boundary condition for the aquifer is specified in the Aquifer Data Group. For Subtitle D applications, only a Gaussian source is allowed which is described in Section 5 of Salhotra et al. (1990). Therefore, default value set in the preprocessor is **Gaussian.** All of the Aquifer Data Group parameters which are not being derived can be assigned either constant values or, in Monte Carlo mode, one of seven distributions (see Table 5-9). Note that an eighth distribution type is available in Monte Carlo mode for the longitudinal, transverse, and vertical dispersivities--the Gelhar distribution. This special distribution is described in Section 6.5.10 and summarized in Table 6-12(a).

5.3.2.5 Unsaturated Zone Flow Data Group--

Table 5-10 shows the parameters in the Unsaturated Zone Flow Data Group. The parameters listed under the heading "Control Parameters" will influence the type of data which can be input in this data group. Thus, these three parameters should be specified first. Each has been assigned a default value which can be changed based on site-specific information. The default values are **1** flow layer, **1** material type, and the use of **van Genuchten** parameters to determine the relationship between relative permeability and water saturation. Note that the number of materials can never be greater than the number of layers. Also note that the same material type can be assigned to more than one layer.

LE 5-8. PARAMETERS IN THE CONTAMINANT SOURCE (SOurce) DATA GROUP

Parameter [units]	Derived	Specified								Comments
Default	C	N	Ln	Exp	U	Log10U	Emp	SB	G	Value
Infiltration rate [m/yr]	–	–	–	–	–	–	–	–		
Area of waste unit [m2yr]	–	–	–	–	–	–	–	–		
Duration of pulse [yr]	Not needed because Subtitle D applications must be steady-state									
Spread of source [m]	–	–	–	–	–	–	–	–	–	
Recharge rate [m/yr]	–	–	–	–	–	–	–	–		
Source Decay constant Set = 0 for Subtitle D applications										0
Initial concentration [mg/l]	–	–	–	–	–	–	–	–		
Length scale [m]	–	–	–	–	–	–	–	–	–	
Width scale [m]	–	–	–	–	–	–	–	–	–	

C	=	Constant	Exp	=	Exponential	Emp	= Empirical
N	=	Normal	U	=	Uniform	SB	= Johnson SB
Ln	=	Lognormal	Log10u	=	Log10Uniform	G	= Gelhar

TABLE 5-9. PARAMETERS IN THE AQUIFER (AQuifer) DATA GROUP

Parameter [units]	Derived	Specified								Default	Comments
	C	N	Ln	Exp	U	$Log_{10}U$	Emp	SB	G	Value	
Depth and Particle Characteristics:											
Particle	■	■	■	■	■	■	■	■	■		
diameter [cm]											Cannot be derived if aquifer porosity is derived.
Porosity [--]	■	■	■	■	■	■	■	■	■		
											Cannot be derived if particle diameter is derived.
Bulk Density [g/cc]	■	■	■	■	■	■	■	■	■		
Aquifer thickness [m]	■	■	■	■	■	■	■	■			
Source thickness [m]	■	■	■	■	■	■	■	■	■		
Type of Source (Gaussian or Patch):								Gaussian			
Hydraulic- and Dispersion-Related Parameters:											
Hydraulic Conductivity [m/yr]	■	■	■	■	■	■	■	■	■		
Hydraulic gradient [--]	■	■	■	■	■	■	■	■			
Seepage velocity [m/yr]	■	■	■	■	■	■	■	■	■		

C = Constant; N = Normal; Ln = Lognormal; Exp = Exponential; U = Uniform; $Log_{10}u$ = Log_{10}Uniform; Emp = Empirical; SB = Johnson SB; G = Gelhar

TABLE 5-9. PARAMETERS IN THE AQUIFER (AQuifer) DATA GROUP

Parameter [units]	Derived	Specified									Comments
		C	N	Ln	Exp	U	$Log_{10}U$	Emp	SB	G	Value
Retardation coeff. [--]		■	■	■	■	■	■	■	■	■	
Longitudinal Dispersivity [m]		■	■	■	■	■	■	■	■ ■	■	
Transverse Dispersivity [m]		■	■	■	■	■	■	■	■ ■	■	
Vertical Dispersivity [m]		■	■	■	■	■	■	■	■ ■	■	
Miscellaneous Parameters:											
Temperature [°C]		■	■	■	■	■	■	■	■		
pH [--]		■	■	■	■	■	■	■	■		
Organic carbon content [fraction]	■	■	■	■	■	■	■	■			

C = Constant; N = Normal; Ln = Lognormal; Exp = Exponential; U = Uniform; $Log_{10}u$ = Log_{10}Uniform; Emp = Empirical; SB = Johnson SB; G = Gelhar

TABLE 5-9. PARAMETERS IN THE AQUIFER (AQuifer) DATA GROUP (concluded)

Parameter [units]	Derived	Specified								Comments
		C	N	Ln	Exp	U	$Log_{10}U$	Emp	SB	G	Value	
Well-Related parameters:												
Receptor distance from site [m]		■	■	■	■	■	■	■	■			
Angle off center Set = 0 for Subtitle D applications.		■									0	
Well vertical Set = 0 for Subtitle D distance [fraction] applications.		■									0	
Flag to reject wells	Not used in Subtitle D outside plume applications.											

Times At Which to Calculate Concentrations: Not used in steady-state applications (steady-state required for Subtitle D applications).

C	=	Constant	Exp	=	Exponential	Emp	=	Empirical
N	=	Normal	U	=	Uniform	SB	=	Johnson SB
Ln	=	Lognormal	$Log_{10}u$	=	Log_{10}Uniform	G	=	Gelhar

TABLE 5-10. PARAMETERS IN THE UNSATURATED ZONE FLOW (Funsat) DATA GROUP

Parameter [units]	Derived	Specified									Default	Comments
	C	N	Ln	Exp	U	$Log_{10}U$	Emp	SB	G	Value		
Control Parameters:												
Number of porous materials		■									1	
van Genuchten or Brooks/Corey flag												van Genuchten
Number of physical flow layers		■									1	
Layer Thickness and Material for Each Layer:												
For 1 layer:												
Depth of the unsat. zone	■	■	■	■	■	■	■	■				
For >1 layer:												
Thickness [m]		■										
For >1 layer:												
Material number of layers		■									0	
Material Properties (for Each Material):												
Saturated hydraulic conductivity [cm/hr]	■	■	■	■	■	■	■	■		■		
Porosity [--]	■	■	■	■	■	■	■	■		■		

C	=	Constant	Exp	=	Exponential	Emp	= Empirical
N	=	Normal	U	=	Uniform	SB	= Johnson SB
Ln	=	Lognormal	$Log_{10}u$	=	Log_{10}Uniform	G	= Gelhar

TABLE 5-10. PARAMETERS IN THE UNSATURATED ZONE FLOW (Funsat) DATA GROUP (concluded)

Parameter [units]	Derived Default	Specified									Comments
		C	N	Ln	Exp	U	$Log_{10}U$	Emp	SB	G	Value
Air entry pressure head [m]		■	■	■	■	■	■	■	■		
Functional Coefficients (for each material):											
Residual water content [--]			■	■	■	■	■	■	■	■	
Brooks and Corey exponent [--]	Not needed if van Genuchten is specified in control parameters	■	■	■	■	■	■	■	■		
Alpha van Genuchten coeff. [1/cm]		■	■	■	■	■	■	■	■		
Beta van Genuchten coeff. [--]		■	■	■	■	■	■	■	■		

C = Constant; N = Normal; Ln = Lognormal; Exp = Exponential; U = Uniform; $Log_{10}u$ = Log_{10}Uniform; Emp = Empirical; SB = Johnson SB; G = Gelhar

When only one layer is modeled, its thickness is equal to the depth of the unsaturated zone and the depth can be assigned a Monte Carlo distribution. When multiple layers are simulated, their thicknesses must be assigned constant values.

Parameters related to material properties and functional relationships must be specified for each material type being modeled. All of these parameters can be assigned a constant value or, in Monte Carlo mode, one of seven Monte Carlo distribution types. The specification of a Monte Carlo distribution requires additional data defining the distribution be input (see Table 5-7). None of the Unsaturated Zone Flow Data Group parameters can be derived.

5.3.2.6 Unsaturated Zone Transport Data Group--

The parameters contained in the Unsaturated Zone Transport Data Group are found in Table 5-11. All of the parameters listed under "Control Parameters" have default values associated with them. The number of layers is defaulted to 1, which corresponds with the number of layers in the Unsaturated Flow Data Group. However, under most conditions the number and thickness of transport layers need not correspond to the number and thickness of flow layers. There are a couple of restrictions: 1) the sum of the transport layer thicknesses must equal the sum of the flow layer thicknesses, and 2) if the depth of the unsaturated zone is assigned a Monte Carlo distribution in the Unsaturated Zone Flow Data Group (see Table 5-10), only one transport layer is allowed.

Unless the modeler has a good understanding of the other "Control Parameters," it is recommended that the default values be used.

For each transport layer being simulated, five parameters need to be specified. The thickness of each layer must be assigned a constant value. The other four parameters can have distributions assigned to them in Monte Carlo mode. Remember that the specification of a Monte Carlo distribution requires that additional data be supplied (see Table 5-7). The longitudinal dispersivity of each layer can be either specified or derived. The derivation of this parameter is described in Section 6.4.2.

TABLE 5-11. PARAMETERS IN THE UNSATURATED ZONE TRANSPORT (Tunsat) DATA GROUP

Parameter [units]	Specified									Derived Default	Comments
	C	N	Ln	Exp	U	$Log_{10}U$	Emp	SB	G	Value	
Control Parameters:											
Number of layers The number of layers need not correspond to the number of layers in Unsaturated Flow.										1	
Scheme for evaluation										Stehfest	
Number of terms for										18	18 is recommended value for scheme Stehfest scheme (the default)
Number of points used for interpolating concs.										3	
Number of Gaussian points										104	
Convolution integral segments										2	
Property Parameters (for Each Transport Layer):											
Thickness of the layer [m]											
Longitudinal dispersivity [m]											
Percent organic matter											
C = Constant N = Normal Ln = Lognormal Exp = Exponential U = Uniform $Log_{10}u$ = Log_{10}Uniform Emp = Empirical SB = Johnson SB G = Gelhar											

TABLE 5-11. PARAMETERS IN THE UNSATURATED ZONE TRANSPORT (Tunsat) DATA GROUP (concluded)

Parameter [units]	Specified										Derived Default	Comments
	C	N	Ln	Exp	U	$Log_{10}U$	Emp	SB	G	Value		
Bulk density [g/cc]	■	■	■	■	■	■	■	■				
Biological decay coeff. [1/yr]	■	■	■	■	■	■	■	■				

C = Constant
Exp = Exponential
Emp = Empirical
N = Normal
U = Uniform
SB = Johnson SB
Ln = Lognormal
$Log_{10}u$ = Log_{10}Uniform
G = Gelhar

SECTION 6

PARAMETER ESTIMATION

This section is intended to provide guidance for estimating parameters required by MULTIMED for Subtitle D land disposal facility applications. It is not intended in any way to be used as a substitute for data collection. Reported values are presented to demonstrate appropriate ranges of values for particular parameters. For easy reference, the parameters are grouped according to the model data group with which they are associated.

The most accurate model results will be obtained from simulations which are based on site-specific data collection. In some cases, however, it is not feasible to measure certain parameters, and satisfactory results have been obtained using estimated values. The code contains the option to internally derive some parameters based on other input parameters. It is recommended that this option be used with caution and only when values from measurements at the site are not available. The parameters that can be derived are identified in this section. The methods used in the code to calculate the derived parameters are summarized briefly in this section, and are discussed in more detail in the MULTIMED model theory documentation (Salhotra et al., 1990).

There are many sources of uncertainty in the prediction of contaminant migration in the subsurface. Utilizing the Monte Carlo option in the model is a method to determine the effect of uncertainty in the model input on the model results. In this option, a parameter is assigned a distribution and its value is then randomly generated. It is often difficult to determine the cumulative probability distribution for a given parameter. These distributions must be determined from a large amount of data, which may not be available. Assuming a parameter probability distribution when the distribution is unknown does not help reduce uncertainty, as the certainty of the output is then a function of the assumed certainty of the input parameter (U.S. EPA, 1988).

Some guidance on determining an appropriate probability density distribution for specific parameters is provided in this section. When possible, tables of descriptive statistics are also given. This information can be ignored if the model is run in a deterministic framework. General information related to the probability distributions and help in determining the number of Monte Carlo runs needed is provided in Section 9 of the MULTIMED model theory documentation (Salhotra et al., 1990).

6.1 CHEMICAL-SPECIFIC PARAMETERS

6.1.1 Overall Chemical Decay Coefficient (Saturated Zone) [1/yr]

This parameter can be derived by the code, which computes it by summing the solid and liquid phase decay coefficients for the saturated zone. Note that the overall chemical decay coefficient does not include biological decay; the biodegradation coefficient must be specified separately. If the value for the overall chemical decay coefficient is specified by the user as a constant or a distribution, the solid and dissolved phase decay coefficients are not needed. In general, the overall decay coefficient for the saturated zone will be smaller in value than for the unsaturated zone.

6.1.2 Solid-Phase and Liquid-Phase Decay Coefficients (Saturated Zone) [1/yr]

These decay coefficients represent the hydrolysis rate constants for the saturated zone. They do not include biological decay, which is discussed in Section 6.1.7. Hydrolysis is a potentially significant elimination pathway for many organic chemicals (Lyman et al., 1982). For compounds which are easily biodegraded, however, hydrolysis may be insignificant relative to biodegradation (see Section 6.1.7). The hydrolysis of organic chemicals can be described as a first-order rate process with respect to the concentration of the organic species (Faust and Gomaa, 1972; Wolfe et al., 1977; 1978) and is dependent on temperature, pH, adsorption, and the presence of organic solvents. Methods for estimating the rate constant for the hydrolysis process are presented in Lyman et al. (1982).

The solid-phase and liquid-phase hydrolysis rate constants can be derived in the code, using input for the acid, base, and neutral hydrolysis rate constants, the reference temperature, and the temperature and pH of the aquifer. The method used by the code to derive these parameters is discussed in Section 5.5.2.1 of the MULTIMED model theory documentation (Salhotra et al., 1990). The use of acid, base, and neutral hydrolysis rates takes into account the strong pH dependence of this process.

If the values of both the solid and dissolved phase decay coefficients are specified by the user, then the saturated transport module does not use the values of the acid, base, and neutral hydrolysis rate constants. They are needed, however, if unsaturated transport and/or surface water transport are also being simulated.

6.1.3 The Acid-Catalyzed and Base-Catalyzed Hydrolysis Rates [ℓ/M-yr] and the Neutral Hydrolysis Rate [1/yr]

These three parameters are used in the code to calculate the overall chemical decay coefficient for the unsaturated, saturated, and surface water modules. The use of these parameters in the unsaturated and saturated transport modules is described in Section 5.5.2.1 of Salhotra et al. (1990). For the surface water module, refer to Section 6.2.1 of the same document. Values of these hydrolysis rate constants are available in a large number of references, including Lyman et al. (1982), Mabey et al. (1982), and Mills et al. (1985a).

6.1.4 Reference Temperature [°C]

The reference temperature is the temperature at which $K^{T}_{a,b}$ and K^{Tr}_{n} were calculated and is normally provided along with the hydrolysis rate constant data.

6.1.5 Distribution Coefficient (Saturated Zone) [ml/g]

Sorption refers to the accumulation of a chemical in the boundary region of a solid-liquid interface (Mills et al., 1985a). Because sorption retards chemical transport in the subsurface, the fate of a chemical is highly dependent on its sorptive characteristics (i.e., the distribution between the sorbed and dissolved phases). MULTIMED assumes that a linear equation can describe the relationship between the equilibrium concentrations of the dissolved and adsorbed phases. The linear relationship requires knowledge of the chemical distribution coefficient, K_d. A number of studies have developed empirical relationships for the partition coefficient. The relationship most suited for relating the chemical distribution coefficient to soil or porous medium properties is discussed in detail by Karickhoff (1984).

In the absence of a user-supplied value, the chemical distribution coefficient for the saturated zone, K_d, can be derived by the code. Hydrophobic binding is assumed to dominate the sorption process and thus, the distribution coefficient is related directly to soil organic carbon content using:

$$K_d = K_{oc} f_{oc} \qquad (6.1)$$

where

K_{oc} = normalized distribution coefficient for organic carbon [mℓ/g]
f_{oc} = organic carbon content in the saturated zone [dimensionless fraction]

The estimation of the normalized distribution coefficient for organic carbon is discussed below.

6.1.6 Normalized Organic Carbon Distribution Coefficient [ml/g]

The normalized organic carbon distribution coefficient, K_{oc}, is used in the code to calculate the chemical distribution coefficient in the unsaturated transport and the surface water modules. It is also used in the saturated transport module when the user chooses to derive the chemical distribution coefficient. There are many published lists of values for K_{oc}. Data are available primarily for pesticides and, to a lesser degree, aromatic and polycyclic aromatic compounds. Lyman et al. (1982) recommend ten different references which contain values of K_{oc}.

If data on K_{oc} are not available for a particular chemical, a value can be estimated from empirical relationships between K_{oc} and some other property of the chemical such as the water solubility, S, the octanol-water partition coefficient, K_{ow}, or the bioconcentration factor for aquatic life, BCF. Lyman et al. (1982) tabulate 12 such regression equations obtained from data sets of different classes of chemicals, and present guidelines for selecting an accurate and applicable equation for a particular chemical. Values for the octanol-water partition coefficient and solubility of priority pollutants are available in many references, including Mabey et al. (1982) and Mills et al. (1985a).

6.1.7 Biodegradation Coefficient (Saturated Zone) [1/yr]

Biodegradation, along with hydrolysis, is one of the decay pathways considered by MULTIMED. For many contaminants, biodegradation is the most significant means of removal from the subsurface environment. However, the biodegradation of chemicals in the environment is complex, depending on a number of variable and/or unknown factors, such as the number of microorganisms present, the availability of oxygen and other nutrients, and the pH and temperature of the system.

A first-order kinetic relationship is normally used to represent biodegradation in the natural environment. It is difficult to estimate the biodegradation coefficient needed

in this relationship. Although attempts have been made to correlate the biodegradability of a compound with its molecular characteristics, such as solubility, these generalizations are applicable only to the specific chemicals investigated, and are not recommended estimation techniques for other chemicals (Lyman et al., 1982). A significant amount of work is needed to validate the extension of these techniques to other chemicals and conditions.

A compilation of laboratory-derived biodegradation rate constants reported in the literature, along with the test conditions when available, is presented in Lyman et al. (1982). The tables include rate constants for several organic compounds in both aqueous environments and soils. However, since these constants were determined under laboratory conditions, they may be inapplicable to a field situation. Additional data are available in Mills et al. (1985a) and Mabey et al. (1982). Care should be taken in extrapolating the results shown in any of these tables to actual environmental situations.

6.2 SOURCE-SPECIFIC PARAMETERS

6.2.1 Recharge Rate [m/yr]

The recharge rate in this model is the net amount of water that percolates directly into the aquifer system outside of the land disposal facility. The recharge is assumed to have no contamination and hence dilutes the groundwater contaminant plume. The recharge rate into the plume can be calculated in a variety of ways. One possibility is to use a model, such as HELP (Hydrologic Evaluation of Landfill Performance) (Schroeder et al., 1984), without any engineering controls (leachate collection system or a liner) to simulate the water balance for natural conditions. Results of such an analysis have been presented by E.C. Jordan Co. (1985, 1987).

6.2.2 Infiltration Rate [m/yr]

The infiltration rate is the net amount of leachate that percolates into the aquifer system from a land disposal facility. Because of the use of engineering controls and the presence of non-native porous materials in the landfill facility, the infiltration rate will typically be different than the recharge rate. However, it can be estimated by similar methods as those discussed for estimation of the recharge rate.

6.2.3 Area of Waste Disposal Unit [m^2]

The area of the waste disposal unit will vary significantly from site to site. The area should be directly measured and input by the user.

6.2.4 Length Scale of Facility [m]

The length of the waste disposal facility should be measured at the site. However, this parameter can be derived by the code. The derivation is based on the assumption that the waste disposal facility has a square shape. Therefore, the code takes the square root of the area:

$$L = (A_w)^{1/2} \qquad (6.2)$$

6.2.5 Width Scale of Facility [m]

The width of the waste disposal facility should be measured at the site. However, as was true for the length scale of the facility (Section 6.2.4), this parameter can be derived by the code, which calculates the width of the facility as the square root of the area.

6.2.6 Initial Concentration at Waste Disposal Facility [mg/l]

When possible, site-specific data should be used. However, the user should bear in mind that concentrations are quite variable over time and thus, a limited set of data may not be representative of conditions at the facility. If data are not available, a conservative approximation would be the solubility of the contaminant in water.

When using the model for the design of Subtitle D facilities, a value of 100 times the Drinking Water Standard can be used (see Section 5.2.4). If the concentration at the well (i.e., point of compliance) is at or below the Drinking Water Standard, the design may prove acceptable. Since the model response is linear with this parameter, it is convenient to use 1.0 mg/l as the initial concentration and to calculate a dilution-attenuation factor (DAF) as discussed in Section 5.4.2.

6.2.7 Source Decay Constant [1/yr]

The source decay constant is used for simulation of an exponentially decreasing (in time) boundary condition (see Section 5.2 of Salhotra et al., 1990). However, the source is assumed to be constant in Subtitle D applications of MULTIMED. Therefore, for Subtitle D applications the preprocessor sets a default value of 0 for the source decay rate.

6.2.8 Duration of Pulse [yr]

The duration of the contaminant pulse is not required in steady-state applications of MULTIMED. Therefore, this parameter does not need to be estimated for Subtitle D applications, which must be steady-state.

6.2.9 Spread of Contaminant Source [m]

The standard deviation of the gaussian source is a measure of the spread of the source. It can be estimated or derived by the code as:

$$\sigma = W/6 \qquad (6.3)$$

where

W = the width scale of the facility--i.e., the dimension of the facility orthogonal to the groundwater flow direction [m]

Dividing by 6 implies that 99.86 percent of the gaussian source spread is within the facility.

6.3 UNSATURATED FLOW PARAMETERS

6.3.1 Saturated Hydraulic Conductivity [cm/hr]

Hydraulic conductivity expresses the ease with which a fluid can be transported through a porous medium and is a function of properties of both the porous medium and the fluid (Mills et al., 1985b). Note that for some materials, such as alluvium, the vertical hydraulic conductivity is significantly smaller than the horizontal hydraulic conductivity. Mills et al. (1985b) state that the ratio of horizontal to vertical conductivity is from 2 to 10 for alluvium and glacial outwash and from 1.5 to 3 for sandstone. In the unsaturated zone module, flow is one-dimensional in the vertical direction, so the vertical hydraulic conductivity should be input. Note that in the saturated zone, the horizontal hydraulic conductivity is required.

One of the most widely-used tables of hydraulic conductivity values is presented in Table 6-1. Note that the use of the values in this table will require a conversion to the units of cm/hr. In addition, descriptive statistics for a variety of soil types are given in Table 6-2. The values for the coefficients of variation in column three are determined from many soils nationwide which fall into each texture group. The coefficient of variation for a single soil is likely to be lower.

The lognormal distribution is likely to be an appropriate probability density function

for saturated hydraulic conductivity (Dean et al., 1989).

Table 6-1 (Graphic)

TABLE 6-2. DESCRIPTIVE STATISTICS FOR SATURATED HYDRAULIC CONDUCTIVITY ($cm\ hr^{-1}$)

Soil Type	Hydraulic Conductivity (K_s)* $\bar{x}$	s	CV	n
Clay**	0.20	0.42	210.3	114
Clay Loam	0.26	0.70	267.2	345
Loam	1.04	1.82	174.6	735
Loamy Sand	14.59	11.36	77.9	315
Silt	0.25	0.33	129.9	88
Silt Loam	0.45	1.23	275.1	1093
Silty Clay	0.02	0.11	453.3	126
Silty Clay Loam	0.07	0.19	288.7	592
Sand	29.70	15.60	52.4	246
Sandy Clay	0.12	0.28	234.1	46
Sandy Clay Loam	1.31	2.74	208.6	214
Sandy Loam	4.42	5.63	127.0	1183

* n = Sample size, $\bar{x}$ = Mean, s = Standard deviation, CV = Coefficient of variation (percent)

** Agricultural soil, less than 60 percent clay

Sources: From Dean et al. (1989),
Original reference Carsel and Parrish (1988).

6.3.2 Unsaturated Zone Porosity [--]

Porosity is a measure of the relative volume of void space in a rock or soil. Porosity is dimensionless and is expressed as a fraction or a percentage. The total porosity of a rock or soil is comprised of primary porosity, which is due to the shape, sorting and packing of the grains in the matrix, and secondary porosity, which is due to phenomena such as cracks and fractures.

MULTIMED requires the effective porosity of the rock or soil as input. The effective porosity is that part of the total porosity which is effective at transmitting water. The effective porosity is typically lower than the total porosity, due to the presence of pores which are not interconnected or the presence of an immobile water film bound to soil grains. In general, laboratory measurements obtain values for total porosity, since effective porosity is difficult to measure directly.

Typical total porosity values for a variety of geologic materials are presented in Table 6-3. Jury (1985) states that a normal distribution is an appropriate probability density function for effective porosity.

6.3.3 Air Entry Pressure Head [m]

The air entry pressure head is the threshold at which air starts to penetrate saturated soil. It is typically a very small negative value for fine-grained materials or zero for coarser soils. Its value can be estimated from the water retention curves of specific soils (Freeze and Cherry, 1979).

6.3.4 Number of Layers, Thickness of Layers [m]

The unsaturated zone extends from the land surface or the bottom of a waste disposal facility to the top of the water table. This distance will vary significantly from site to site. An estimate of this depth can be determined from water level measurements in the area of the site.

TABLE 6-3. TOTAL POROSITY OF VARIOUS MATERIALS

Material	No. of Analyses	Range	Arithmetic Mean
Igneous Rocks			
Weathered granite	8	0.34-0.57	0.45
Weathered gabbro	4	0.42-0.45	0.43
Basalt	94	0.03-0.35	0.17
Sedimentary Materials			
Sandstone	65	0.14-0.49	0.34
Siltstone	7	0.21-0.41	0.35
Sand (fine)	243	0.26-0.53	0.43
Sand (coarse)	26	0.31-0.46	0.39
Gravel (fine)	38	0.25-0.38	0.34
Gravel (coarse)	15	0.24-0.36	0.28
Silt	281	0.34-0.61	0.46
Clay	74	0.34-0.57	0.42
Limestone	74	0.07-0.56	0.30
Metamorphic Rocks			
Schist	18	0.04-0.49	0.38

Sources: From Mercer et al. (1982),
McWhorter and Sunada (1977),
Original reference Morris and Johnson, (1967).

In MULTIMED, the unsaturated zone can be modeled with up to 20 layers which have distinct physical characteristics. Information about the layers, which should be relatively homogeneous and distinguishable from adjacent layers, must be determined on a site-specific basis. Note that more than one layer can be assigned the same material properties. When one homogeneous layer is modeled, the layer thickness is equal to the depth of the unsaturated zone and the depth of the unsaturated zone can have a Monte Carlo distribution assigned to it. Refer to Section 6.4.1 for more information.

6.3.5 Residual Water Content [--]

The residual water content is that amount of the total water content which can not be removed from the soil, even under large suction pressure, because it adheres to the soil grains. Descriptive statistics for residual water content for a variety of types of soils are presented in Table 6-4. In addition, the residual water content for a large number of soils can be estimated using the interactive computer program, DBAPE, which is a soils data base analyzer and parameter estimator (Imhoff et al., 1990). DBAPE is available from the U.S. EPA Center for Environmental Assessment Modeling (CEAM) at the Environmental Research Laboratory in Athens, Georgia.

6.3.6 Brooks and Corey Exponent [--]

The Brooks and Corey exponent, n, is an empirical parameter used in an equation which describes the relationship between relative permeability and water saturation (see Section 3.2 of the MULTIMED model theory documentation (Salhotra et al., 1990)). The exponent can be determined from experimental data for a soil's capillary pressure-desaturation curve. Brooks and Corey (1966) present experimental results for several porous media. The porous media investigated by the authors had values of n ranging from 3.27 for glass beads to 4.11 for a silt loam. Soils composed of single-grained material with no secondary porosity (e.g., sands) tend to have smaller exponent values. Soils with structure or secondary porosity have larger exponent values.

In MULTIMED, the relationship between relative permeability and water saturation may be described using either the Brooks and Corey (1966) or the van Genuchten (1976) relationship (see Section 3 of Salhotra et al. (1990)). The Brooks and Corey exponent is not required when the use of the van Genuchten relationship is specified in the input. However, both the Brooks and Corey exponent and the van Genuchten parameters are required when the use of the Brooks and Corey relationship is specified.

6.3.7 Van Genuchten Parameters, α [1/cm]; β [--]

In the code, the relationship between relative permeability and water saturation may be described using either the Brooks and Corey (1966) or the van Genuchten (1976) relationship. However, the pressure head versus water saturation relationship is described using van Genuchten parameters (see Section 3 of the MULTIMED model theory documentation (Salhotra et al., 1990)). Therefore, the van Genuchten parameters must be input to simulate unsaturated flow in the code. Descriptive statistics for these empirical parameters have been reported by Carsel and Parrish (1988) for a variety of soil types (see Table 6-5).

TABLE 6-4. DESCRIPTIVE STATISTICS FOR SATURATION WATER CONTENT (θ_s) AND RESIDUAL WATER CONTENT (θ_r)

	Saturation Water Content (θ_s)				Residual Water Content (θ_r)			
	Statistic*							
Soil Type	$\bar{x}$	s	CV	n	x	s	CV	n
Clay**	0.38	0.09	24.1	400	0.068	0.034	49.9	353
Clay Loam	0.41	0.09	22.4	364	0.095	0.010	10.1	363
Loam	0.43	0.10	22.1	735	0.078	0.013	16.5	735
Loamy Sand	0.41	0.09	21.6	315	0.057	0.015	25.7	315
Silt	0.46	0.11	17.4	82	0.034	0.010	29.8	82
Silt Loam	0.45	0.08	18.7	1093	0.067	0.015	21.6	1093
Silty Clay	0.36	0.07	19.6	374	0.070	0.023	33.5	371
Silty Clay Loam	0.43	0.07	17.2	641	0.089	0.009	10.6	641
Sand	0.43	0.06	15.1	246	0.045	0.010	22.3	246
Sandy Clay	0.38	0.05	13.7	46	0.100	0.013	12.9	46
Sandy Clay Loam	0.39	0.07	17.5	214	0.100	0.006	6.0	214
Sandy Loam	0.41	0.09	21.0	1183	0.065	0.017	26.6	1183

* n = Sample size, $\bar{x}$ = Mean, s = standard deviation, CV = coefficient of variation (percent)

** Agricultural soil, less than 60 percent clay.

Source: Dean et al. (1989)
Original source Carsel and Parrish (1988)

6.4 UNSATURATED TRANSPORT PARAMETERS

6.4.1 Number of Layers, Thickness of Layers

The number of layers specified for transport in the unsaturated zone will depend on the specific conditions present at the site. Layers should represent zones that are relatively homogeneous with regard to the properties affecting transport and that can be distinguished from adjacent layers by changes in these properties. Note that the number and thickness of layers specified in the transport module need not correspond to the number and thickness of layers in the unsaturated flow module (see Section 6.3.4). However, the sum of the individual layer thicknesses in the two modules must equal each other (i.e., the total depth of the unsaturated zone must agree in the two modules). If the depth of the unsaturated zone is assigned a Monte Carlo distribution in the unsaturated flow module, then only one unsaturated transport layer is allowed.

Table 6-5. DESCRIPTIVE STATISTICS FOR VAN GENUCHTEN WATER RETENTION MODEL PARAMETERS, α, β, and γ (Carsel and Parrish 1988)

	Parameter α, cm^{-1}				Parameter β				Parameter γ			
Soil Type	$\bar{X}$	SD	CV	N	$\bar{X}$	SD	CV	N	$\bar{X}$	SD	CV	N
Clay[a]	0.008	0.012	160.3	400	1.09	0.09	7.9	400	0.08	0.07	82.7	400
Clay Loam	0.019	0.015	77.9	363	1.31	0.09	7.2	364	0.24	0.06	23.5	364
Loam	0.036	0.021	57.1	735	1.56	0.11	7.3	735	0.36	0.05	13.5	735
Loamy Sand	0.124	0.043	35.2	315	2.28	0.27	12.0	315	0.56	0.04	7.7	315
Silt	0.016	0.007	45.0	88	1.37	0.05	3.3	88	0.27	0.02	8.6	88
Silt Loam	0.020	0.012	64.7	1093	1.41	0.12	8.5	1093	0.29	0.06	19.9	1093
Silty Clay	0.005	0.005	113.6	126	1.09	0.06	5.0	374	0.09	0.05	51.7	374
Silty Clay Loam	0.010	0.006	61.5	641	1.23	0.06	5.0	641	0.19	0.04	21.5	641
Sand	0.145	0.029	20.3	246	2.68	0.29	20.3	246	0.62	0.04	6.3	246
Sandy Clay	0.027	0.017	61.7	46	1.23	0.10	7.9	46	0.18	0.06	34.7	46
Sandy Clay Loam	0.059	0.038	64.6	214	1.48	0.13	8.7	214	0.32	0.06	53.0	214
Sandy Loam	0.075	0.037	49.4	1183	1.89	0.17	9.2	1183	0.47	0.05	10.1	1183

$\bar{X}$ = Mean, SD = Standard Deviation, CV = Coefficient of Variation (percent), N = Sample size

[a] Agricultural Soil, Clay 60 percent

6.4.2 Longitudinal Dispersivity of Each Layer [m]

Hydrodynamic dispersion refers to the spreading and mixing caused by molecular diffusion and mechanical dispersion (Freeze and Cherry, 1979). For many field problems, molecular diffusion is small relative to mechanical dispersion and can be ignored. Molecular diffusion is not considered in MULTIMED, which calculates the longitudinal dispersion coefficient as the product of the seepage velocity and longitudinal (α_L) dispersivity. Note that longitudinal dispersion is the dispersion in the predominant direction of flow, which is vertical in the unsaturated zone.

Dispersivity is a difficult parameter to determine. Table 6-6 provides a compilation of dispersivity values appropriate for the unsaturated transport module. Research has shown that the values for longitudinal dispersivity are scale dependent. In an unsaturated transport layer, if a value for the longitudinal dispersivity is not input, the user can specify that the parameter be derived. The equation used in the model to calculate dispersivity is based on regression analysis of the data in Table 6-6. The following relationship between dispersivity and the depth of the unsaturated zone, L, was developed:

$$\alpha_v = 0.02 + 0.022L, \qquad R^2 = 66\% \tag{6.4}$$

To avoid excessively high values of dispersivity for deep unsaturated zones, a maximum dispersivity of 1.0 m is used.

Distributional properties for longitudinal dispersivity are unknown (Dean et al., 1989).

6.4.3 Percent Organic Matter [--]

Guidance in estimating the percent organic matter is provided in Table 6-7. Values are given for the four Hydrologic Soil Groups and for four ranges of depth. From Appendix B of the users manual for PRZM, Release I (Carsel et al., 1984) or from Section 4 of the SCS National Engineering Handbook (Soil Conservation Service, 1972), the hydrologic soil group for the particular soil that is in the area under consideration can be found. There are four different soil classifications (A, B, C, and D), and they are in the order of decreasing percolation potential and increasing slope and runoff potential. Soil characteristics associated with each hydrologic group are as follows:

Group A: Deep sand, deep loess, aggregated silts, minimum infiltration of 0.76 - 1.14 (cm hr^{-1})

Group B: Shallow loess, sandy loam, minimum infiltration 0.38 - 0.76 (cm hr^{-1})

Group C: Clay loams, shallow sandy loam, soils low in organic content, and soils usually high in clay, minimum infiltration 0.13 - 0.38 (cm hr^{-1})

Group D: Soils that swell significantly when wet, heavy plastic clays, some saline soils, minimum infiltration 0.03 - 0.13 (cm hr^{-1})

TABLE 6-6. COMPILATION OF FIELD DISPERSIVITY VALUES *

Author	Type of Experiment	Vertical Scale of Experiment (m)	Longitudinal Dispersivity α_v (m)
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

* From Dean et al. (1989),
Original reference Gelhar et al. (1985).

TABLE 6-7. DESCRIPTIVE STATISTICS AND DISTRIBUTION MODEL FOR ORGANIC MATTER (PERCENT BY WEIGHT)

Stratum	Sample	Original Data				Distribution Model	
(m)	Size	Mean	Median	s.d.	CV (%)	Mean	s.d.
Class A							
0.0-0.3	162	0.86	0.62	0.79	92	-4.53	0.96
0.3-0.6	162	0.29	0.19	0.34	114	-5.72	0.91
0.6-0.9	151	0.15	0.10	0.14	94	-6.33	0.83
0.9-1.2	134	0.11	0.07	0.11	104	-6.72	0.87
Class B							
0.0-0.3	1135	1.3	1.1	0.87	68	-4.02	0.76
0.3-0.6	1120	0.50	0.40	0.40	83	-5.04	0.77
0.6-0.9	1090	0.27	0.22	0.23	84	-5.65	0.75
0.9-1.2	1001	0.18	0.14	0.16	87	-6.10	0.78
Class C							
0.0-0.3	838	1.45	1.15	1.12	77	-3.95	0.79
0.3-0.6	822	0.53	0.39	0.61	114	-5.08	0.84
0.3-0.9	780	0.28	0.22	0.27	96	-5.67	0.83
0.9-1.2	672	0.20	0.15	0.21	104	-6.03	0.88
Class D							
0.0-0.3	638	1.34	1.15	0.87	66	-4.01	0.73
0.3-0.6	617	0.65	0.53	0.52	80	-4.79	0.78
0.6-0.9	558	0.41	0.32	0.34	84	-5.29	0.82
0.9-1.2	493	0.29	0.22	0.31	105	-5.65	0.86

CV = coefficient of variation
s.d. = standard deviation
Source: Dean et al. (1989), Original reference Carsel et al. (1988)
[a] Johnson s_B transformation is used for all cases in this table.

Carsel et al. (1988) state that a Johnson SB distribution is most appropriate for the data in Table 6-7. Note that the percent organic matter typically decreases with depth. More detailed data on percent organic matter are available through the interactive computer program DBAPE discussed in Section 6.3.5 (Imhoff et al., 1990).

If the percent organic matter is not known, but the fractional organic carbon content is given, the following equation can be used to estimate the percent organic matter:

$$f_{om} = 172.4\ f_{oc} \qquad (6.5)$$

where

f_{oc} = fractional organic carbon content [dimensionless]
f_{om} = percent organic matter [dimensionless]
172.4 = conversion factor from percent organic matter content to fractional organic carbon content

6.4.4 Bulk Density of Soil for Layer [g/cc]

Bulk density can be defined as the mass of a unit volume of dry soil (Mercer et al., 1982). The soil bulk density directly influences the retardation of solutes and is related to the structure and texture of a soil. The bulk density of soils typically range between 1.3 and 2.0 g/cc, but Mercer et al. (1982) state that the bulk density can be as low as 0.3 g/cc for soils high in organics or aluminum and iron hydroxides. Representative values for five different types of soils are shown in Table 6-8. In addition, values of bulk density for a large number of soils can be obtained from DBAPE, discussed in Section 6.3.5 (Imhoff et al., 1990).

Descriptive statistics for bulk density are given in Table 6-9 for the four Hydrologic Soil Groups (A, B, C, and D) and for four ranges of depth. (A brief description of the soil groups in given in Section 6.4.3.) The most appropriate probability density distribution for bulk density is typically a normal distribution (Jury, 1985).

6.4.5 Biological Decay Coefficient [1/yr]

Estimation of the biodegradation rate constant is discussed in Section 6.1.7.

6.5 AQUIFER-SPECIFIC PARAMETERS

6.5.1 Aquifer Porosity [--]

Porosity is also discussed in Section 6.5.1 and values of porosity for various materials are given in Table 6-3. It is an important parameter, influencing the velocity and retardation of contaminants transported in an aquifer (Mills et al., 1985b). In the absence of a user-specified distribution for the aquifer porosity, it can be derived by the code. It is calculated from the particle diameter using the following empirical relationship (Federal Register Vol. 51, No. 9, p. 1649, 1986):

TABLE 6-8. MEAN BULK DENSITY (g/cm^3) FOR FIVE SOIL TEXTURAL CLASSIFICATIONS[a,b]

Soil Texture	Mean Value	Range Reported
Silt Loams	1.32	0.86 - 1.67
Clay and Clay Loams	1.30	0.94 - 1.54
Sandy Loams	1.49	1.25 - 1.76
Gravelly Silt Loams	1.22	1.02 - 1.58
Loams	1.42	1.16 - 1.58
All Soils	1.35	0.86 - 1.76

[a] Baes, C.F., III and R.D. Sharp. 1983. A Proposal for Estimation of Soil Leaching Constants for Use in Assessment Models. J. Environ. Qual. 12(1):17-28 (Original reference).

[b] From Dean et al. (1989)

$$\theta = 0.261 - 0.0385 \ln(d) \qquad (6.6)$$

where d is the mean particle diameter [cm].

6.5.2 Particle Diameter [cm]

The particle diameter can be determined by methods such as sieve analysis (Freeze and Cherry, 1979). Table 6-10 shows the range of soil particle sizes for a variety of soil materials. If the porosity is known, the particle diameter can be derived using Equation 6.6. Note that both porosity and particle diameter can not be derived in the same simulation (i.e., at least one must be input by the user).

6.5.3 Bulk Density [g/cc]

Bulk density is discussed in Section 6.4.4 and Tables 6-8 and 6-9 provide data on the bulk density of soils. However, the bulk density of aquifer materials may differ significantly from that of soils. Therefore, data on the ranges of bulk density for various geologic material are presented in Table 6-11.

If site-specific data are not available, the bulk density of the saturated zone can be derived by the model using an exact relationship between porosity, particle density and the bulk density (Freeze and Cherry, 1979). Assuming the particle density to be 2.65 g/cc, this relationship can be expressed as:

Table 6-9. DESCRIPTIVE STATISTICS FOR BULK DENSITY (g cm^{-3})

Stratum (m)	Sample Size	Mean	Median	s.d.	CV (%)
Class A					
0.0-0.3	40	1.45	1.53	0.24	16.2
0.3-0.6	44	1.50	1.56	0.23	15.6
0.6-0.9	38	1.57	1.55	0.16	10.5
0.9-1.2	34	1.58	1.59	0.13	8.4
Class B					
0.0-0.3	459	1.44	1.45	0.19	13.5
0.3-0.6	457	1.51	1.53	0.19	12.2
0.6-0.9	438	1.56	1.57	0.19	12.3
0.9-1.2	384	1.60	1.60	0.21	12.9
Class C					
0.0-0.3	398	1.46	1.48	0.22	15.0
0.3-0.6	395	1.58	1.59	0.23	14.5
0.6-0.9	371	1.64	1.65	0.23	14.2
0.9-1.2	326	1.67	1.68	0.23	14.0
Class D					
0.0-0.3	259	1.52	1.53	0.24	15.9
0.3-0.6	244	1.63	1.66	0.26	16.0
0.6-0.9	214	1.67	1.72	0.27	16.3
0.9-1.2	180	1.65	1.72	0.28	17.0

CV = coefficient of variation
s.d. = standard deviation

Sources: From Dean et al. (1989),
Original reference Carsel et al. (1988).

TABLE 6-10. RANGE OF SOIL PARTICLE SIZES FOR VARIOUS MATERIALS

Class name	Size Range: Millimeters	Size Range: Inches	Approximate Sieve Mesh Openings: Tyler	Approximate Sieve Mesh Openings: United States Standard
Very large boulders	4,096-2,048	160-80		
Large boulders	2,048-1,024	80-40		
Medium boulders	1,024-512	40-20		
Small boulders	512-256	20-10		
Large cobbles	256-128	10-5		
Small cobbles	128-64	5-2.5		
Very coarse gravel	64-32	2.5-1.3		
Coarse gravel	32-16	1.3-0.6		
Medium gravel	16-8	0.6-0.3	2-1/2	
Fine gravel	8-4	0.3-0.16	5	5
Very fine gravel	4-2	0.16-0.08	9	10
Very coarse sand	2.000-1.000		16	18
Coarse sand	1.000-0.500		32	35
Medium sand	0.500-0.250		60	60
Fine sand	0.250-0.125		115	120
Very fine sand	0.125-0.062		250	230
Coarse silt	0.062-0.031			
Medium silt	0.031-0.016			
Fine silt	0.016-0.008			
Very fine silt	0.008-0.004			
Coarse clay	0.004-0.0020			
Medium clay	0.0020-0.0010			
Fine clay	0.0010-0.0005			
Very fine clay	0.0005-0.00024			

Reference: Modified from Vanoni (1975).

$$\rho_b = 2.65(1 - \theta) \qquad (6.7)$$

where ρ_b = the bulk density of the soil [g/cc].

6.5.4 Aquifer Thickness [m]

The estimation of the thickness of the aquifer is site-specific, and should be based on available geologic data.

6.5.5 Source Thickness (Mixing Zone Depth) [m]

Percolation of water through the facility (and unsaturated zone, if it exists) results in the development of a contaminant plume below the facility (see Figure 6.1). The thickness, H, of this plume depends on the vertical dispersivity of the media. If a value for H is not known, it can be derived in the model using the following relationship:

TABLE 6-11. RANGE AND MEAN VALUES OF DRY BULK DENSITY FOR VARIOUS GEOLOGIC MATERIALS

Material	Range (g/cm^3)	Mean (g/cm^3)
Clay	1.18-1.72	1.49
Silt	1.01-1.79	1.38
Sand, fine	1.13-1.99	1.55
Sand, medium	1.27-1.93	1.69
Sand, coarse	1.42-1.94	1.73
Gravel, fine	1.60-1.99	1.76
Gravel, medium	1.47-2.09	1.85
Gravel, coarse	1.69-2.08	1.93
Loess	1.25-1.62	1.45
Eolian sand	1.33-1.70	1.58
Till, predominantly silt	1.61-1.91	1.78
Till, predominantly sand	1.69-2.12	1.88
Till, predominantly gravel	1.72-2.12	1.91
Glacial drift, predominantly silt	1.11-1.66	1.38
Glacial drift, predominantly sand	1.36-1.83	1.55
Glacial drift, predominantly gravel	1.47-1.78	1.60
Sandstone, fine grained	1.34-2.32	1.76
Sandstone, medium grained	1.50-1.86	1.68
Siltstone	1.35-2.12	1.61
Claystone	1.37-1.60	1.51
Shale	2.20-2.72	2.53
Limestone	1.21-2.69	1.94
Dolomite	1.83-2.20	2.02
Granite, weathered	1.21-1.78	1.50
Gabbro, weathered	1.67-1.77	1.73
Basalt	1.99-2.89	2.53
Schist	1.42-2.69	1.76

Reference: Morris and Johnson (1967); Mills et al. (1985b)

Figure 6.1

$$H = (2\alpha_v L)^{\frac{1}{2}} + B\left(1 - \exp\left(-\frac{LQ_f}{V_s \theta B}\right)\right) \quad (6.8)$$

where

α_v = the vertical dispersivity [m]
L = the length scale of the facility--i.e., the dimension of the facility parallel to the flow direction [m] (if L is not known, an estimate can be obtained from Equation 6.2)
B = the thickness of the saturated zone [m]
V_s = one-dimensional, uniform seepage velocity in the x direction [m/yr]
Q_f = percolation rate [m/yr]

In Equation 6.8 the first term represents the thickness of the plume due to vertical dispersion and the second term represents the thickness of the plume due to the vertical velocity below the facility resulting from percolation. While implementing this alternative, the code checks that the computed value of the thickness of the source, H, is not greater than the thickness of the aquifer, B. If it is, the source thickness is set equal to the aquifer thickness.

6.5.6 Hydraulic Conductivity [m/yr]

Hydraulic conductivity estimates should be based on site-specific data collection, such as piezometer tests (bail tests or slug tests) and/or pumping tests. Some typical hydraulic conductivity values for various materials are shown in Tables 6-1 and 6-2 and discussed in Section 6.3.1. Note that the units of hydraulic conductivity are m/yr in the saturated zone, but cm/hr elsewhere in the code.

An alternative, though often a poor one, is to allow the code to derive a value for hydraulic conductivity. The code uses an approximate functional relationship, the Kozeny-Carman equation (Bear 1979):

$$K = \frac{\rho g}{\mu} \frac{\theta^3}{(1-\theta)^2} \frac{d^2}{1.8} \quad (6.9)$$

where

K = the hydraulic conductivity [cm/s]
ρ = the density of water [kg/m^3]
g = acceleration due to gravity [m/s^2]
μ = the dynamic viscosity of water [$N\text{-}s/m^2$]
d = mean particle diameter [cm]

In Equation 6.9, the constant 1.8 includes a unit conversion factor. Both the density of water, ρ, and the dynamic viscosity of water, μ, are functions of temperature and are computed using regression equations presented in CRC (1981). Note that at 15°C, the value of $[\rho g/1.8\mu]$ is about 478.

6.5.7 Hydraulic Gradient [m/m]

The hydraulic gradient is the change in water level elevation over a given distance. In general, it is a function of the local topography, groundwater recharge volume and location, and the volume and location of groundwater withdrawals. Further, it may also be related to the porous media properties.

The gradient can often be estimated from water level measurements in the area surrounding the site or from a map of water table or potentiometric surface elevations. The average gradient under natural conditions should be input in the model. Therefore estimates should not include the effect of pumping. The data used to estimate the hydraulic gradient can also be used to determine the direction of groundwater flow.

6.5.8 Groundwater Seepage Velocity [m/yr]

The groundwater velocity is needed to quantify transport by advection. Because groundwater velocities are difficult to measure directly, they are often determined indirectly, using the fact that seepage velocity is related to the aquifer properties through Darcy's Law. Assuming a uniform, saturated porous medium, the seepage velocity can be expressed as:

$$V_s = KS/\theta \qquad (6.10)$$

where

K = the hydraulic conductivity of the formation [m/yr]
S = the hydraulic gradient [m/m]

MULTIMED allows the user to derive the seepage velocity by means of Equation 6.10 instead of directly entering a value.

Note that the hydraulic conductivity of the aquifer is used by the code only to calculate the seepage velocity. Therefore, if the groundwater seepage velocity is specified by the user, the hydraulic conductivity will not be used.

6.5.9 Retardation Coefficient [--]

The retardation factor is used to determine the retardation, due to adsorption, of a contaminant relative to the bulk mass of water transporting the contaminant (Freeze and Cherry, 1979). In addition to delaying the arrival time of a contaminant at a receptor, retardation together with dispersion can lower the peak concentration. In MULTIMED, the retardation factor can be input directly or derived by the code using:

$$R_s = 1 + \rho_b K_d/\theta \qquad (6.11)$$

where

ρ_b = bulk density [g/cc]
K_d = contaminant distribution coefficient [cc/g]
θ = saturation water content [--]

Estimation of the bulk density, distribution coefficient, and saturation water content has been discussed in earlier sections. Note that a value of one for the retardation coefficient means that the contaminant does not interact with the solid phase, but acts as a conservative tracer. An example of a conservative tracer is chloride.

6.5.10 Longitudinal, Transverse and Vertical Dispersivities [m]

The aquifer longitudinal (α_L), transverse (α_T), and vertical (α_v) dispersivities are used in the model to calculate hydrodynamic dispersion (i.e., the spreading and mixing caused by mechanical dispersion). The spreading of a contaminant caused by molecular diffusion is assumed to be small relative to mechanical dispersion and is ignored in the model. The estimation of longitudinal dispersivity in the unsaturated zone is discussed in Section 6.4.2. Note that the longitudinal dispersivity is oriented in the vertical direction for the unsaturated zone, while it is oriented in the horizontal direction for the saturated zone.

The values for dispersivity are difficult to determine. Research has shown that the values for these parameters are strongly scale dependent (EPRI, 1985). This can be seen in Figure 6.2. In general, dispersion is determined by adjusting the dispersivity values until modeling results match historical data (Mercer et al., 1982).

In the absence of user-specified values, the model allows two alternatives for deriving the aquifer dispersivities. Alternative one is based on values presented in Gelhar and Axness (1981). Dispersivities are calculated as a fraction of the distance to the downgradient receptor well, as follows:

$$\alpha_L = 0.1\ x_r \tag{6.12}$$

$$\alpha_T = \alpha_L/3.0 \tag{6.13}$$

$$\alpha_v = 0.056\alpha_L \tag{6.14}$$

where x_r is the distance to the receptor well [m]. This option is summarized in Table 6-12(a).

Alternative two allows a probabilistic formulation for the longitudinal dispersivity as shown in Tables 6-12(a) and 6-12(b) [Gelhar (personal communication), 1986]. The longitudinal dispersivity is assumed to be uniform within each of the three intervals shown in Table 6-12(b). Note that these values of longitudinal dispersivity shown are based on a receptor well distance of 152.4 m. For other distances, the following equation is used:

$$\alpha_L(x_r) = \alpha_L(x_r = 152.4)(x_r/152.4)^{0.5} \tag{6.15}$$

The transverse and vertical dispersivity are assumed to have the following values:

Figure 6.2

TABLE 6-12(a). ALTERNATIVES FOR INCLUDING DISPERSIVITIES IN THE SATURATED ZONE MODULE

Dispersivity	Alternative 1 Existing Values	Alternative 2 Gelhar's Recommendation
α_L [m] Formulation	0.1 x_r	Probabilistic (See Table 5-3(b))
α_T [m]	0.333 α_L	$\alpha_L/8$
α_V [m]	0.056 α_L	$\alpha_L/160$
α_L/α_T	3	8
α_L/α_V	approx. 18	160

TABLE 6-12(b). PROBABILISTIC REPRESENTATION OF LONGITUDINAL DISPERSIVITY FOR A DISTANCE OF 152.4 m

Class	1	2	3
α_L (m)	0.1-1	1-10	10-100
Probability	0.1	0.6	0.3
Cumulative Probability	0.1	0.7	1.0

$$\alpha_T = \alpha_L/8 \quad (6.16)$$

$$\alpha_v = \alpha_L/160 \quad (6.17)$$

The distributional properties for the longitudinal and transverse dispersivities are unknown (Dean et al., 1989).

6.5.11 Aquifer Temperature [°C]

This parameter is site-specific and should be measured at the site. Note that MULTIMED does not take into account any seasonal variation in temperature in the uppermost portions of the aquifer. Instead, an average value should be used. The average temperature of shallow groundwater in the United States is shown in Figure 6.3.

6.5.12 pH [pH units]

The pH values of groundwater in the United States typically range between 6.0 and 8.5. However, values as high as 11.0 for alkali-spring water and as low as 1.8 for acid hot-spring water have been determined (Mercer et al., 1982). The pH can be measured from groundwater samples in the field. For some aquifers, data may be available from the U.S. Geological Survey, the U.S. Environmental Protection Agency, or from state and local agencies.

6.5.13 Organic Carbon Content (Fraction) [--]

The fractional organic carbon content can be estimated from the percent organic matter by the following relationship:

$$f_{oc} = f_{om}/172.4 \quad (6.18)$$

where

f_{oc} = fractional organic carbon content [dimensionless]
f_{om} = percent organic matter [dimensionless]
172.4 = conversion factor from percent organic matter content to fractional organic carbon content

Information about the percent organic matter in soils is provided in Section 6.4.3. Typically the value of the percent organic matter (and hence, the fractional organic carbon content) is smaller for an aquifer than for near-surface soils.

6.5.14 Well Distance from Site [m], Angle off Center [degrees], and Well Vertical Distance [m]

A schematic of the receptor well location relative to the waste facility was presented in Figure 6.1. The location of the well is determined by specifying the radial distance to the well, the angle between the plume centerline and the radial location of the well measured counterclockwise and the depth of penetration of the well. The well screen depth is specified as the fraction (i.e., a value between 0 and 1) of the total aquifer thickness and is measured downward from the water table. The well is assumed to have a single opening at the depth specified. The code uses the input to calculate the cartesian coordinates of the well location as discussed in Section 5.2.3.

For Subtitle D applications of the model, a conservative approach is required. Thus, the well is assumed to be located on the contaminant plume centerline (i.e., the angle off center is fixed at zero degrees) and the well vertical distance is also fixed at zero (i.e., the contaminant concentration is predicted at the water table).

Figure 6.3

SECTION 7

EXAMPLE PROBLEMS

Three example problems are presented in this section. These problems are designed to demonstrate the application of MULTIMED to a variety of scenarios which might be encountered while studying Subtitle D facilities. Example 1 is a deterministic, steady-state simulation of transport in the saturated zone. The second example is identical to Example 1, but includes flow and transport in the unsaturated zone. This example is included in the deterministic tutorial for the preprocessor, PREMED, and can be accessed from the opening screen of the preprocessor by typing <@DETER.LOG> (do not type the brackets). Example 3 is similar to Example 2, but it is run in Monte-Carlo mode. This example is the same as the input generated by the Monte Carlo tutorial, which is accessed from the preprocessor opening screen by typing <@MONTE.LOG>.

Because new versions of the MULTIMED code may be released after the publication of this document, the results presented in this section may differ from the result obtained from using the input generated by the tutorials. Therefore, these examples should not be viewed as validation data sets. Input and output for model validation are distributed with the code.

Note that the scenarios represented by these simulations are hypothetical, and are not intended to resemble any actual sites. The values used in these example problems are not EPA-recommended values for use in MULTIMED.

7.1 EXAMPLE 1

7.1.1 The Hypothetical Scenario

A well which supplies drinking water to a small community is located 152 meters directly downgradient from a waste disposal facility. The members of the community want to predict the effect of the waste disposal facility on the water quality in the well.

The bottom of the waste disposal facility is located just above the water table. Therefore, simulation of flow and transport in the unsaturated zone is unnecessary, and only saturated transport is simulated.

One contaminant has been selected by the community for simulation, based on its unusual persistence in the subsurface environment. This contaminant is not biodegradable, and has an overall chemical decay coefficient which is so small it can be assumed to be zero (this is a conservative approach). The normalized

distribution coefficient for the contaminant is also assumed to be zero, so the chemical will not be removed from the groundwater by the process of adsorption. For convenience in calculating the dilution attenuation factor (DAF), discussed in Section 5.2.4, the concentration of the contaminant at the bottom of the facility is assumed to be 1.00 mg/l. This source concentration is constant in time. The area of the waste disposal site is approximately 400 m^2 and it is square in shape. The infiltration rate into the aquifer beneath the facility is .007 m/yr, and the recharge rate into the aquifer downgradient of the facility is slightly higher at .0076 m/yr. No temporal variability in these rates has been observed.

The aquifer is 78.6 meters thick and the hydraulic gradient within the aquifer is constant at 0.0306. The estimated longitudinal dispersivity in the aquifer is 160 m, the transverse dispersivity is 15.2 m and the vertical dispersivity is 8 m. The fraction of organic carbon in the aquifer is .00315. The pH of the groundwater in the aquifer is typical of many groundwaters in the United States and has been measured to be 6.20. The average annual temperature in the aquifer is 14.4 °C.

The lack of temporal variability in this system indicates that a steady-state simulation is appropriate. Furthermore, the values of the parameters are known with a high degree of certainty, so a deterministic simulation was selected.

7.1.2 Input

MULTIMED input for Example 1 is shown in Table 7-1. It consists of the title for the Example 1 simulation, followed by several data groups. The values assigned to specific parameters are clearly labeled for all of the data groups except the General data group. The parameters in the General Data Group and the format of the entire input sequence are discussed in Appendix A.
Since only the saturated transport module is used in this example, the General Data Group is followed by three data groups: the Chemical, Source and Aquifer Specific Variable Data. In these data groups, the name of the input parameter and the units for the parameter are in the left hand column. The values listed under "Distribution" indicate whether the parameter is to be derived from other parameters (-1 or -2) or read from the input sequence (0). Since this is a deterministic simulation, only the values listed in the "Mean" column will be used by the model (the standard deviation, and the minimum and maximum limits are applicable only in a Monte Carlo simulation).

All of the Chemical Specific Parameters used by MULTIMED are listed in the input file. However, not all of these parameters are used in the Example 1 simulation. A discussion of which parameters are required by the saturated zone transport module can be found in Section 5.3. To avoid obtaining values for unnecessary parameters when developing an input sequence for MULTIMED, refer to Section 5.3, which discusses the parameters required for specific modules, and Section 6, which discusses the estimation and/or derivation of these parameters.

Values for some parameters may be listed as -999. These parameters are undefined. Files generated by the preprocessor list some of the parameters which are not used by the code as -999. PREMED will check that all of the necessary values for a particular simulation have been defined before saving an input file. If a value of -999 appears in the input sequence for a parameter which <u>is</u> required by the code, this parameter will be listed as "Undefined", and must be specified to complete the input sequence for use in MULTIMED. The specification of "Undefined" parameters is clearly demonstrated in the PREMED tutorials.

TABLE 7-1. INPUT SEQUENCE FOR EXAMPLE 1.

```
4444444444
```

TABLE 7-1. INPUT SEQUENCE FOR EXAMPLE 1 (concluded).

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
```

```
SOURCE SPECIFIC VARIABLE DATA
ARRAY VALUES
***         SOURCE SPECIFIC VARIABLES
```

*** VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	STD DEV	LIMITS MIN	MAX
1 Infiltration rate	(m/yr)	0	0.700E-02	-999.	0.100E-09	0.100E+11
2 Area of waste disp unit	(m^2)	0	400.	-999.	0.100E-01	-999.
3 Duration of pulse	(yr)	0	-999.	-999.	0.100E-08	-999.
4 Spread of contaminant srce	(m)	-1	-999.	-999.	0.100E-08	0.100E+11
5 Recharge rate	(m/yr)	0	0.760E-02	-999.	0.100E-09	0.100E+11
6 Source decay constant	(1/yr)	0	0.000E+00	-999.	0.000E+00	-999.
7 Init conc at landfill	(mg/l)	0	1.00	-999.	0.000E+00	-999.
8 Length scale of facility	(m)	-1	-999.	-999.	0.100E-08	0.100E+11
9 Width scale of facility	(m)	-1	-999.	-999.	0.100E-08	0.100E+11

```
END ARRAY

END SOURCE SPECIFIC VARIABLE DATA

AQUIFER SPECIFIC VARIABLE DATA
ARRAY VALUES
***         AQUIFER SPECIFIC VARIABLES
```

*** VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	STD DEV	LIMITS MIN	MAX
1 Particle diameter	(cm)	0	0.630E-03	-999.	0.100E-08	100.
2 Aquifer porosity		-2	-999.	-999.	0.100E-08	0.990
3 Bulk density	(g/cc)	-2	-999.	-999.	0.100E-01	5.00
4 Aquifer thickness	(m)	0	78.6	-999.	0.100E-08	0.100E+06
5 Mixing zone depth	(m)	-1	-999.	-999.	0.100E-08	0.100E+06
6 Hydraulic conductivity	(m/yr)	-2	-999.	-999.	0.100E-06	0.100E+09
7 Hydraulic Gradient		0	0.306E-01	-999.	0.100E-07	-999.
8 Grndwater seep velocity	(m/yr)	-2	-999.	-999.	0.100E-09	0.100E+09
9 Retardation coefficient		-1	-999.	-999.	1.00	0.100E+09
10 Longitudinal dispersivity	(m)	0	160.	-999.	0.100E-02	0.100E+05
11 Transverse dispersivity	(m)	0	15.2	-999.	0.100E-02	0.100E+05
12 Vertical dispersivity	(m)	0	8.00	-999.	0.100E-02	0.100E+05
13 Temperature of aquifer	(C)	0	14.4	-999.	0.000E+00	100.
14 pH		0	6.20	-999.	0.300	14.0
15 Organic carbon content	(fract)	0	0.315E-02	-999.	0.100E-05	1.00
16 Receptor distance from site	(m)	0	152.	-999.	1.00	-999.
17 Angle off center	(degree)	0	0.000E+00	-999.	0.000E+00	360.
18 Well vert dist from water tabl		0	0.000E+00	-999.	0.000E+00	1.00

```
END ARRAY

END AQUIFER SPECIFIC VARIABLE DATA
END ALL DATA
```

7.1.3 Output

The output for example 1 consists the main output file, the SAT.OUT file, and files with a *.VAR extension, which are not shown. For deterministic simulations, the *.VAR files echo the values of the constant parameters and list the values calculated by the code for the derived parameters. Table 7-2 presents the main output file, which consists of an echo of the input and the predicted contaminant concentration at the well. The SAT.OUT file, shown in Table 7-3, lists the predicted contaminant concentration at the well.

7.2 EXAMPLE 2

7.2.1 The Hypothetical Scenario

The second example is identical to the first with one exception: the water table is located at a depth of 6.1 meters below the bottom of the waste disposal facility. Therefore, unsaturated flow and transport must also be simulated.

In this example, the unsaturated zone consists of one homogeneous layer with the following known values for material and transport properties. The saturated hydraulic conductivity is .017 cm/hr, the porosity is 0.43 and the bulk density is 1.67 g/cm^3. The percent organic matter is 0.026 and the Brooks and Corey exponent is 0.5. The van Genuchten parameters, α and β, which describe the relationship between the pressure head and water saturation, are .009 and 1.23, respectively. The residual water content is .088 and the longitudinal dispersivity is .4 m.

7.2.2 Input

The chemical, source, and aquifer specific parameters are the same as those described in Example 1. However, simulation of the unsaturated zone requires additional data groups in the input file including soil moisture parameters and unsaturated zone transport parameters. The input for Example 2 is shown in Table 7-4.

7.2.3 Output

The output for Example 2 is similar to that described for Example 1. In addition to the main output file, shown in Table 7-5, the SAT.OUT file, presented in Table 7-6, and the *.VAR files, two additional files, VFLOW.OUT and VTRNSPT.OUT, are created. VFLOW.OUT contains output for the Unsaturated Zone Flow Module, including the depth of each node and the Darcy velocity, water saturation, and head at each node. (Note that the number and location of nodes is determined by the MULTIMED code.) VTRNSPT.OUT lists the steady-state concentration at the water table.

TABLE 7-2. OUTPUT FILE FOR EXAMPLE 1.

```
4444444444
```

TABLE 7-2. OUTPUT FILE FOR EXAMPLE 1.

CHEMICAL SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Solid phase decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Dissolved phase decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Overall chemical decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Acid catalyzed hydrolysis rate	l/M-yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Neutral hydrolysis rate constant	1/yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Base catalyzed hydrolysis rate	l/M-yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Reference temperature	C	CONSTANT	25.0	0.000E+00	0.000E+00	100.
Normalized distribution coefficient	ml/g	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Distribution coefficient	--	DERIVED	0.219	0.000E+00	0.000E+00	0.100E+11
Biodegradation coefficient (sat. zone)	1/yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Air diffusion coefficient	cm2/s	CONSTANT	0.000E+00	0.645E-02	0.000E+00	10.0
Reference temperature for air diffusion	C	CONSTANT	0.000E+00	0.000E+00	0.000E+00	100.
Molecular weight	g/M	CONSTANT	-999.	0.000E+00	0.000E+00	-999.
Mole fraction of solute	--	CONSTANT	-999.	0.100E-01	0.100E-08	1.00
Vapor pressure of solute	mm Hg	CONSTANT	-999.	0.230E-01	0.000E+00	100.
Henry`s law constant	atm-m^3/M	CONSTANT	-999.	0.000E+00	0.100E-09	1.00
RFD value for drinking water	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00
ADIF value for fish consumption	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00
CCC for aquatic organisms	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00

1

SOURCE SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Infiltration rate	m/yr	CONSTANT	0.700E-02	-999.	0.100E-09	0.100E+11
Area of waste disposal unit	m^2	CONSTANT	400.	-999.	0.100E-01	-999.
Duration of pulse	yr	CONSTANT	-999.	-999.	0.100E-08	-999.
Spread of contaminant source	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Recharge rate	m/yr	CONSTANT	0.760E-02	-999.	0.100E-09	0.100E+11
Source decay constant	1/yr	CONSTANT	0.000E+00	-999.	0.000E+00	-999.
Initial concentration at landfill	mg/l	CONSTANT	1.00	-999.	0.000E+00	-999.
Length scale of facility	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Width scale of facility	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Near field dilution		CONSTANT	0.000E+00	0.000E+00	0.000E+00	0.000E+00

1

(continued)

TABLE 7-2. OUTPUT FILE FOR EXAMPLE 1 (concluded).
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

AQUIFER SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Particle diameter	cm	CONSTANT	0.630E-03	-999.	0.100E-08	100.
Aquifer porosity	--	DERIVED	-999.	-999.	0.100E-08	0.990
Bulk density	g/cc	DERIVED	-999.	-999.	0.100E-01	5.00
Aquifer thickness	m	CONSTANT	78.6	-999.	0.100E-08	0.100E+06
Source thickness (mixing zone depth)	m	DERIVED	-999.	-999.	0.100E-08	0.100E+06
Conductivity (hydraulic)	m/yr	DERIVED	-999.	-999.	0.100E-06	0.100E+09
Gradient (hydraulic)		CONSTANT	0.306E-01	-999.	0.100E-07	-999.
Groundwater seepage velocity	m/yr	DERIVED	-999.	-999.	0.100E-09	0.100E+09
Retardation coefficient	--	DERIVED	-999.	-999.	1.00	0.100E+09
Longitudinal dispersivity	m	CONSTANT	160.	-999.	0.100E-02	0.100E+05
Transverse dispersivity	m	CONSTANT	15.2	-999.	0.100E-02	0.100E+05
Vertical dispersivity	m	CONSTANT	8.00	-999.	0.100E-02	0.100E+05
Temperature of aquifer	C	CONSTANT	14.4	-999.	0.000E+00	100.
pH	--	CONSTANT	6.20	-999.	0.300	14.0
Organic carbon content (fraction)		CONSTANT	0.315E-02	-999.	0.100E-05	1.00
Well distance from site	m	CONSTANT	152.	-999.	1.00	-999.
Angle off center	degree	CONSTANT	0.000E+00	-999.	0.000E+00	360.
Well vertical distance	m	CONSTANT	0.000E+00	-999.	0.000E+00	1.00

CONCENTRATION AFTER SATURATED ZONE MODEL 0.5736E-03

TABLE 7-3. SAT.OUT FILE FOR EXAMPLE 1.

```
44444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
1

                    STEADY STATE SATURATED ZONE TRANSPORT RESULTS
 AT 0.1000E+04 YEARS, CONCENTRATION IS 0.5736E-03
```

TABLE 7-4. INPUT SEQUENCE FOR EXAMPLE 2.

```
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
Test input sequence for MULTIMED.
Example 2.


GENERAL DATA

***  CHEMICAL NAME FORMAT(80A1)
DEFAULT CHEMICAL

***    ISOURC                                ROUTE      NT        IYCHK   PALPH       APPTYP
***OPTION   OPTAIR  RUN                 MONTE    ISTEAD     IOPEN     IZCHK     LANDF   COMPLETE
    2    0    0     DETERMINISTIC        1    1    1    1    0    0    0 90.0    0    2    1


***   XST

END GENERAL

CHEMICAL SPECIFIC VARIABLE DATA
ARRAY VALUES
***      CHEMICAL SPECIFIC VARIABLES

***            VARIABLE NAME                UNITS                DISTRIBUTION   PARAMETERS              LIMITS
***                                                                                MEAN      STD DEV    MIN      MAX
 ***************************************************************************************************************************
 1 Solid phase decay coeff (1/yr)                                    -1       0.000E+00 0.000E+00 0.000E+00 0.100E+11
 2 Diss phase decay coeff (1/yr)                                     -1       0.000E+00 0.000E+00 0.000E+00 0.100E+11
 3 Overall chem dcy coeff (1/yr)                                     -1       0.000E+00 0.000E+00 0.000E+00 0.100E+11
 4 Acid cataly hydrol rte(1/M-yr)                                     0       0.000E+00 0.000E+00 0.000E+00 -999.
 5 Neutral hydrol rate cons(1/yr)                                     0       0.000E+00 0.000E+00 0.000E+00 -999.
 6 Base cataly hydrol rte(1/M-yr)                                     0       0.000E+00 0.000E+00 0.000E+00 -999.
 7 Reference temperature (C)                                          0        25.0     0.000E+00 0.000E+00  100.
 8 Normalized distrib coeff(ml/g)                                     0       0.000E+00 0.000E+00 0.000E+00 -999.
 9 Distribution coefficient                                          -2       0.219     0.000E+00 0.000E+00 0.100E+11
10 Biodegrad coef(sat zone)(1/yr)                                     0       0.000E+00 0.000E+00 0.000E+00 -999.
11 Air diffusion coeff (cm2/s)                                        0       0.000E+00 0.645E-02 0.000E+00  10.0
12 Ref temp for air diffusion (C)                                     0       0.000E+00 0.000E+00 0.000E+00  100.
13 Molecular weight (g/mole)                                          0       -999.     0.000E+00 0.000E+00 -999.
14 Mole fraction of solute                                            0       -999.     0.100E-01 0.100E-08  1.00
15 Solute vapor pressure (mm Hg)                                      0       -999.     0.230E-01 0.000E+00  100.
16 Henry`s law cons (atm-m^3/M)                                       0       -999.     0.000E+00 0.100E-09  1.00
17 Not in use                                                         0        1.00     0.000E+00 0.000E+00  1.00
18 Not in use                                                         0        1.00     0.000E+00 0.000E+00  1.00
19 Not in use                                                         0        1.00     0.000E+00 0.000E+00  1.00
END ARRAY

END CHEMICAL SPECIFIC VARIABLE DATA
```

(continued)

TABLE 7-4. INPUT SEQUENCE FOR EXAMPLE 2.

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
SOURCE SPECIFIC VARIABLE DATA
ARRAY VALUES
***         SOURCE SPECIFIC VARIABLES

***            VARIABLE NAME                 UNITS                DISTRIBUTION   PARAMETERS              LIMITS
***                                                                                  MEAN       STD DEV    MIN       MAX
 ********************************************************************************************************************************
 1 Infiltration rate (m/yr)                                                  0      0.700E-02 -999.      0.100E-09 0.100E+11
 2 Area of waste disp unit (m^2)                                             0       400.     -999.      0.100E-01 -999.
 3 Duration of pulse (yr)                                                    0      -999.     -999.      0.100E-08 -999.
 4 Spread of contaminant srce (m)                                           -1      -999.     -999.      0.100E-08 0.100E+11
 5 Recharge rate (m/yr)                                                      0      0.760E-02 -999.      0.100E-09 0.100E+11
 6 Source decay constant (1/yr)                                              0      0.000E+00 -999.      0.000E+00 -999.
 7 Init conc at landfill (mg/l)                                              0       1.00     -999.      0.000E+00 -999.
 8 Length scale of facility (m)                                             -1      -999.     -999.      0.100E-08 0.100E+11
 9 Width scale of facility (m)                                              -1      -999.     -999.      0.100E-08 0.100E+11
END ARRAY

END SOURCE SPECIFIC VARIABLE DATA


VFL   UNSATURATED FLOW MODEL PARAMETERS


CONTROL PARAMETERS
***    DUMMY      NMAT       KPROP      DUMMY     NVFLAY
         7          1          2          1          1

END CONTROL PARAMETERS
MATERIAL NUMBER FOR EACH LAYER
  6.10           1
END MATERIAL PARAMETERS
SATURATED MATERIAL PROPERTY PARAMETERS
ARRAY VALUES
***   SATURATED MATERIAL   VARIABLES

***            VARIABLE NAME                 UNITS                DISTRIBUTION   PARAMETERS              LIMITS
***                                                                                  MEAN       STD DEV    MIN       MAX
 ********************************************************************************************************************************
 1 Sat hydraulic conduct (cm/hr)                                             0      0.170E-01 -999.      0.100E-10 0.100E+05
 2 Unsaturated zone porosity                                                 0      0.430     -999.      0.100E-08 0.990
 3 Air entry pressure head (m)                                               0      0.000E+00 -999.      0.000E+00 -999.
 4 Depth of the unsat zone (m)                                               0       6.10     -999.      0.100E-08 -999.
END ARRAY

END MATERIAL  1
END
```

(continued)

TABLE 7-4. INPUT SEQUENCE FOR EXAMPLE 2.

```
44444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

SOIL MOISTURE PARAMETERS
***   FUNCTIONAL COEFFICIENTS
ARRAY VALUES
***   FUNCTIONAL COEFFICIE VARIABLES

***            VARIABLE NAME                UNITS                DISTRIBUTION   PARAMETERS              LIMITS
***                                                                                MEAN       STD DEV    MIN       MAX
 ***************************************************************************************************************************
 1 Residual water content                                                  0       0.880E-01 -999.      0.100E-08  1.00
 2 Brooks and Corey exponent, EN                                           0       0.500     -999.      0.000E+00  10.0
 3 ALFA van Genuchten coefficient                                          0       0.900E-02 -999.      0.000E+00  1.00
 4 BETA Van Genuchten coefficient                                          0        1.23     -999.       1.00      5.00
END ARRAY

END MATERIAL  1
END
END UNSATURATED FLOW



VTP    UNSATURATED TRANSPORT MODEL
CONTROL PARAMETERS
***   NLAY      DUMMY      IADU      ISOL        N       NTEL     NGPTS       NIT      DUMMY     DUMMY
         1         20         1         1       18          3       104         2          1         1
***  WTFUN
     1.200


END CONTROL PARAMETERS
TRANSPORT PARAMETER
ARRAY VALUES
***   UNSATURATED TRANSPOR VARIABLES

***            VARIABLE NAME                UNITS                DISTRIBUTION   PARAMETERS              LIMITS
***                                                                                MEAN       STD DEV    MIN       MAX
 ***************************************************************************************************************************
 1 Thickness of layer (m)                                                  0        6.10     -999.      0.100E-08 -999.
 2 Longit disper of layer (m)                                              0       0.400     -999.      0.000E+00 0.100E+05
 3 Percent organic matter                                                  0       0.260E-01 -999.      0.000E+00  100.
 4 Bulk dens of soil layer (g/cc)                                          0        1.67     -999.      0.100E-01  5.00
 5 Biological decay coeff (1/yr)                                           0       0.000E+00 -999.      0.000E+00 -999.
END ARRAY

END LAYER  1
END UNSATURATED TRANSPORT PARAMETERS
END TRANSPORT MODEL
```

(continued)

TABLE 7-4. INPUT SEQUENCE FOR EXAMPLE 2 (concluded).
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

AQUIFER SPECIFIC VARIABLE DATA
ARRAY VALUES
*** AQUIFER SPECIFIC VARIABLES

***	VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	STD DEV	LIMITS MIN	MAX
1	Particle diameter (cm)		0	0.630E-03	-999.	0.100E-08	100.
2	Aquifer porosity		-2	-999.	-999.	0.100E-08	0.990
3	Bulk density (g/cc)		-2	-999.	-999.	0.100E-01	5.00
4	Aquifer thickness (m)		0	78.6	-999.	0.100E-08	0.100E+06
5	Mixing zone depth (m)		-1	-999.	-999.	0.100E-08	0.100E+06
6	Hydraulic conductivity (m/yr)		-2	-999.	-999.	0.100E-06	0.100E+09
7	Hydraulic Gradient		0	0.306E-01	-999.	0.100E-07	-999.
8	Grndwater seep velocity (m/yr)		-2	-999.	-999.	0.100E-09	0.100E+09
9	Retardation coefficient		-1	-999.	-999.	1.00	0.100E+09
10	Longitudinal dispersivity (m)		0	160.	-999.	0.100E-02	0.100E+05
11	Transverse dispersivity (m)		0	15.2	-999.	0.100E-02	0.100E+05
12	Vertical dispersivity (m)		0	8.00	-999.	0.100E-02	0.100E+05
13	Temperature of aquifer (C)		0	14.4	-999.	0.000E+00	100.
14	pH		0	6.20	-999.	0.300	14.0
15	Organic carbon content (fract)		0	0.315E-02	-999.	0.100E-05	1.00
16	Receptor distance from site(m)		0	152.	-999.	1.00	-999.
17	Angle off center (degree)		0	0.000E+00	-999.	0.000E+00	360.
18	Well vert dist from water tabl		0	0.000E+00	-999.	0.000E+00	1.00

END ARRAY

END AQUIFER SPECIFIC VARIABLE DATA

END ALL DATA

TABLE 7-5. MAIN OUTPUT FILE FOR EXAMPLE 2.

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
```

U. S. E N V I R O N M E N T A L P R O T E C T I O N A G E N C Y

E X P O S U R E A S S E S S M E N T

M U L T I M E D I A M O D E L

VERSION 3.3, DECEMBER 1988

Developed by Phillip Mineart and Atul Salhotra of
Woodward-Clyde Consultants, Oakland, California
In cooperation with:
Hydrogeologic, Inc., Herndon, Virginia,
Geotrans, Inc., Herndon, Virginia,
and
Aqua Terra Consultants, Mountain View, California

```
1
 Run options
 --- -------

 Subtitle D landfill application.
 Chemical simulated is DEFAULT CHEMICAL


 Option Chosen                          Saturated and unsaturated zone models
 Run was                                DETERMIN
 Infiltration input by user
 Run was steady-state
 Reject runs if Y coordinate outside plume
 Reject runs if Z coordinate outside plume
 Gaussian source used in saturated zone model
1
1
 UNSATURATED ZONE FLOW MODEL PARAMETERS
 (input parameter description and value)
 NP     - Total number of nodal points                240
 NMAT   - Number of different porous materials          1
 KPROP  - Van Genuchten or Brooks and Corey             2
 IMSHGN - Spatial discretization option                 1
        1


 OPTIONS CHOSEN
 ------- ------
 Brooks and Corey functional coefficients
 User defined coordinate system
1
```

(continued)

TABLE 7-5. MAIN OUTPUT FILE FOR EXAMPLE 2.

Layer information

LAYER NO.	LAYER THICKNESS	MATERIAL PROPERTY
1	6.10	1

DATA FOR MATERIAL 1

VADOSE ZONE MATERIAL VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
Saturated hydraulic conductivity	cm/hr	CONSTANT	0.170E-01	-999.	0.100E-10	0.100E+05
Unsaturated zone porosity	--	CONSTANT	0.430	-999.	0.100E-08	0.990
Air entry pressure head	m	CONSTANT	0.000E+00	-999.	0.000E+00	-999.
Depth of the unsaturated zone	m	CONSTANT	6.10	-999.	0.100E-08	-999.

1

UNSATURATED ZONE TRANSPORT MODEL PARAMETERS

NLAY	- Number of different layers used		1
NTSTPS	- Number of time values concentration calc		20
DUMMY	- Not presently used		1
ISOL	- Type of scheme used in unsaturated zone		1
N	- Stehfest terms or number of increments		18
NTEL	- Points in Lagrangian interpolation		3
NGPTS	- Number of Gauss points		104
NIT	- Convolution integral segments		2
IBOUND	- Type of boundary condition		1
ITSGEN	- Time values generated or input		1
TMAX	- Max simulation time	--	0.0
WTFUN	- Weighting factor	--	1.2

OPTIONS CHOSEN

Stehfest numerical inversion algorithm
Nondecaying continuous source
Computer generated times for computing concentrations

1

(continued)

TABLE 7-5. MAIN OUTPUT FILE FOR EXAMPLE 2.

DATA FOR LAYER 1

VADOSE TRANSPORT VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
Thickness of layer	m	CONSTANT	6.10	-999.	0.100E-08	-999.
Longitudinal dispersivity of layer	m	CONSTANT	0.400	-999.	0.000E+00	0.100E+05
Percent organic matter	--	CONSTANT	0.260E-01	-999.	0.000E+00	100.
Bulk density of soil for layer	g/cc	CONSTANT	1.67	-999.	0.100E-01	5.00
Biological decay coefficient	1/yr	CONSTANT	0.000E+00	-999.	0.000E+00	-999.

1

CHEMICAL SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
Solid phase decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Dissolved phase decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Overall chemical decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Acid catalyzed hydrolysis rate	1/M-yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Neutral hydrolysis rate constant	1/yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Base catalyzed hydrolysis rate	1/M-yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Reference temperature	C	CONSTANT	25.0	0.000E+00	0.000E+00	100.
Normalized distribution coefficient	ml/g	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Distribution coefficient	--	DERIVED	0.219	0.000E+00	0.000E+00	0.100E+11
Biodegradation coefficient (sat. zone)	1/yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Air diffusion coefficient	cm2/s	CONSTANT	0.000E+00	0.645E-02	0.000E+00	10.0
Reference temperature for air diffusion	C	CONSTANT	0.000E+00	0.000E+00	0.000E+00	100.
Molecular weight	g/M	CONSTANT	-999.	0.000E+00	0.000E+00	-999.
Mole fraction of solute	--	CONSTANT	-999.	0.100E-01	0.100E-08	1.00
Vapor pressure of solute	mm Hg	CONSTANT	-999.	0.230E-01	0.000E+00	100.
Henry`s law constant	atm-m^3/M	CONSTANT	-999.	0.000E+00	0.100E-09	1.00
RFD value for drinking water	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00
ADIF value for fish consumption	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00
CCC for aquatic organisms	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00

1

(continued)

TABLE 7-5. MAIN OUTPUT FILE FOR EXAMPLE 2 (concluded).
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

SOURCE SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Infiltration rate	m/yr	CONSTANT	0.700E-02	-999.	0.100E-09	0.100E+11
Area of waste disposal unit	m^2	CONSTANT	400.	-999.	0.100E-01	-999.
Duration of pulse	yr	CONSTANT	-999.	-999.	0.100E-08	-999.
Spread of contaminant source	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Recharge rate	m/yr	CONSTANT	0.760E-02	-999.	0.100E-09	0.100E+11
Source decay constant	1/yr	CONSTANT	0.000E+00	-999.	0.000E+00	-999.
Initial concentration at landfill	mg/l	CONSTANT	1.00	-999.	0.000E+00	-999.
Length scale of facility	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Width scale of facility	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Near field dilution		CONSTANT	0.000E+00	0.000E+00	0.000E+00	0.000E+00

1

AQUIFER SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Particle diameter	cm	CONSTANT	0.630E-03	-999.	0.100E-08	100.
Aquifer porosity	--	DERIVED	-999.	-999.	0.100E-08	0.990
Bulk density	g/cc	DERIVED	-999.	-999.	0.100E-01	5.00
Aquifer thickness	m	CONSTANT	78.6	-999.	0.100E-08	0.100E+06
Source thickness (mixing zone depth)	m	DERIVED	-999.	-999.	0.100E-08	0.100E+06
Conductivity (hydraulic)	m/yr	DERIVED	-999.	-999.	0.100E-06	0.100E+09
Gradient (hydraulic)		CONSTANT	0.306E-01	-999.	0.100E-07	-999.
Groundwater seepage velocity	m/yr	DERIVED	-999.	-999.	0.100E-09	0.100E+09
Retardation coefficient	--	DERIVED	-999.	-999.	1.00	0.100E+09
Longitudinal dispersivity	m	CONSTANT	160.	-999.	0.100E-02	0.100E+05
Transverse dispersivity	m	CONSTANT	15.2	-999.	0.100E-02	0.100E+05
Vertical dispersivity	m	CONSTANT	8.00	-999.	0.100E-02	0.100E+05
Temperature of aquifer	C	CONSTANT	14.4	-999.	0.000E+00	100.
pH	--	CONSTANT	6.20	-999.	0.300	14.0
Organic carbon content (fraction)		CONSTANT	0.315E-02	-999.	0.100E-05	1.00
Well distance from site	m	CONSTANT	152.	-999.	1.00	-999.
Angle off center	degree	CONSTANT	0.000E+00	-999.	0.000E+00	360.
Well vertical distance	m	CONSTANT	0.000E+00	-999.	0.000E+00	1.00

CONCENTRATION AFTER SATURATED ZONE MODEL 0.5736E-03

TABLE 7-6. SAT.OUT FILE FOR EXAMPLE 2.

```
44444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
1

                    STEADY STATE SATURATED ZONE TRANSPORT RESULTS
  AT 0.1000E+04 YEARS, CONCENTRATION IS 0.5736E-03
```

7.3 EXAMPLE 3

7.3.1 The Hypothetical Scenario

The third example is similar to Example 2. The difference is that Example 3 is run in Monte-Carlo mode instead of in a deterministic framework. In this example, spatial variability is observed in the measured values for two parameters, which introduces uncertainty into the model. Therefore, it is necessary to utilize the Monte Carlo option in MULTIMED.

In Example 3, all but three of the parameter values are constant or derived and are identical to those in Example 2. The three parameters have some uncertainty associated with their values. Thus, they are described in terms of probability density functions which represent the uncertainty in the parameter value. The theory behind the Monte Carlo analysis technique, and the probability density distributions included in MULTIMED, are discussed in Section 9 of Salhotra et al. (1990).

The three uncertain parameters in Example 3 are the unsaturated zone hydraulic conductivity (cm/hr), the unsaturated zone porosity, and the aquifer pH. In this example, the probability density distribution is lognormal for the hydraulic conductivity, normal for the unsaturated zone porosity, and uniform for the aquifer pH. The normal and lognormal distributions both require specification of a mean, standard deviation, and minimum and maximum limits. The uniform distribution requires only the minimum and maximum limits of values. Values for these parameters are shown in Table 7-7.

7.3.2 Input

The input sequence for Example 3 is shown in Table 7-8. It is identical to the input file for Example 2 except for changes in the General Data Group related to running the model in a Monte Carlo framework, and differences in the input for the three parameters which have been assigned Monte Carlo distributions.

TABLE 7-7. MONTE CARLO DISTRIBUTION VALUES IN EXAMPLE 3

Parameter	Distribution	Mean	Standard Deviation	Limits Min.	Limits Max.
Saturated hydraulic conductivity (cm/hr) for the unsaturated zone	Lognormal	.017	.020	.001	.250
Unsaturated zone porosity	Normal	.330	.100	.200	.450
Aquifer pH	Uniform	NA	NA	5.80	6.90

TABLE 7-8. INPUT SEQUENCE FOR EXAMPLE 3.
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

Example 3 input
Subtitle D application

GENERAL DATA

*** CHEMICAL NAME FORMAT(80A1)
DEFAULT CHEMICAL

***	ISOURC				ROUTE		NT		IYCHK		PALPH		APPTYP	
***OPTION		OPTAIR	RUN	MONTE		ISTEAD		IOPEN		IZCHK		LANDF		COMPLETE
2	0	0	MONTE	500	1	1	1	1	0	0	90.0	0	2	1

*** XST

END GENERAL

CHEMICAL SPECIFIC VARIABLE DATA
ARRAY VALUES
*** CHEMICAL SPECIFIC VARIABLES

***	VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	STD DEV	LIMITS MIN	MAX
1	Solid phase decay coeff (1/yr)		-1	0.000E+00	0.000E+00	0.000E+00	0.100E+11
2	Diss phase decay coeff (1/yr)		-1	0.000E+00	0.000E+00	0.000E+00	0.100E+11
3	Overall chem dcy coeff (1/yr)		-1	0.000E+00	0.000E+00	0.000E+00	0.100E+11
4	Acid cataly hydrol rte(1/M-yr)		0	0.000E+00	0.000E+00	0.000E+00	-999.
5	Neutral hydrol rate cons(1/yr)		0	0.000E+00	0.000E+00	0.000E+00	-999.
6	Base cataly hydrol rte(1/M-yr)		0	0.000E+00	0.000E+00	0.000E+00	-999.
7	Reference temperature (C)		0	25.0	0.000E+00	0.000E+00	100.
8	Normalized distrib coeff(ml/g)		0	140.	0.000E+00	0.000E+00	-999.
9	Distribution coefficient		-2	0.219	0.000E+00	0.000E+00	0.100E+11
10	Biodegrad coef(sat zone)(1/yr)		0	0.000E+00	0.000E+00	0.000E+00	-999.
11	Air diffusion coeff (cm2/s)		0	0.000E+00	0.645E-02	0.000E+00	10.0
12	Ref temp for air diffusion (C)		0	0.000E+00	0.000E+00	0.000E+00	100.
13	Molecular weight (g/mole)		0	-999.	0.000E+00	0.000E+00	-999.
14	Mole fraction of solute		0	-999.	0.100E-01	0.100E-08	1.00
15	Solute vapor pressure (mm Hg)		0	-999.	0.230E-01	0.000E+00	100.
16	Henry`s law cons (atm-m^3/M)		0	-999.	0.000E+00	0.100E-09	1.00
17	Not in use		0	1.00	0.000E+00	0.000E+00	1.00
18	Not in use		0	1.00	0.000E+00	0.000E+00	1.00
19	Not in use		0	1.00	0.000E+00	0.000E+00	1.00

END ARRAY

END CHEMICAL SPECIFIC VARIABLE DATA

(continued)

TABLE 7-8. INPUT SEQUENCE FOR EXAMPLE 3.

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
```

```
SOURCE SPECIFIC VARIABLE DATA
ARRAY VALUES
***         SOURCE SPECIFIC VARIABLES

***             VARIABLE NAME                 UNITS                DISTRIBUTION    PARAMETERS              LIMITS
***                                                                                    MEAN       STD DEV     MIN       MAX
 ********************************************************************************************************************************
 1 Infiltration rate (m/yr)                                                  0       0.700E-02 -999.      0.100E-09 0.100E+11
 2 Area of waste disp unit (m^2)                                             0        400.     -999.      0.100E-01 -999.
 3 Duration of pulse (yr)                                                    0       -999.     -999.      0.100E-08 -999.
 4 Spread of contaminant srce (m)                                           -1       -999.     -999.      0.100E-08 0.100E+11
 5 Recharge rate (m/yr)                                                      0       0.160E-01 -999.      0.100E-09 0.100E+11
 6 Source decay constant (1/yr)                                              0       0.000E+00 -999.      0.000E+00 -999.
 7 Init conc at landfill (mg/l)                                              0        1.00     -999.      0.000E+00 -999.
 8 Length scale of facility (m)                                             -1       -999.     -999.      0.100E-08 0.100E+11
 9 Width scale of facility (m)                                              -1       -999.     -999.      0.100E-08 0.100E+11
END ARRAY

END SOURCE SPECIFIC VARIABLE DATA


VFL   UNSATURATED FLOW MODEL PARAMETERS


CONTROL PARAMETERS
***     DUMMY      NMAT      KPROP      DUMMY     NVFLAY
          7          1          1          1          1


END CONTROL PARAMETERS
SATURATED MATERIAL PROPERTY PARAMETERS
ARRAY VALUES
***    SATURATED MATERIAL    VARIABLES

***             VARIABLE NAME                 UNITS                DISTRIBUTION    PARAMETERS              LIMITS
***                                                                                    MEAN       STD DEV     MIN       MAX
 ********************************************************************************************************************************
 1 Sat hydraulic conduct (cm/hr)                                             2       0.170E-01 0.200E-01 0.100E-03 0.250
 2 Unsaturated zone porosity                                                 1       0.330     0.100     0.200     0.450
 3 Air entry pressure head (m)                                               0       0.000E+00 -999.     0.000E+00 -999.
 4 Depth of the unsat zone (m)                                               0        6.10     -999.     0.100E-08 -999.
END ARRAY

END MATERIAL  1
END
```

(continued)

TABLE 7-8. INPUT SEQUENCE FOR EXAMPLE 3.

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
```

```
SOIL MOISTURE PARAMETERS
***   FUNCTIONAL COEFFICIENTS
ARRAY VALUES
***   FUNCTIONAL COEFFICIE VARIABLES

***            VARIABLE NAME                UNITS               DISTRIBUTION   PARAMETERS            LIMITS
***                                                                              MEAN      STD DEV    MIN       MAX
 ********************************************************************************************************************
 1 Residual water content                                          0       0.880E-01 -999.     0.100E-08  1.00
 2 Brooks and Corey exponent, EN                                   0       0.500     -999.     0.000E+00  10.0
 3 ALFA van Genuchten coefficient                                  0       0.900E-02 -999.     0.000E+00  1.00
 4 BETA Van Genuchten coefficient                                  0        1.23     -999.      1.00      5.00
END ARRAY

END MATERIAL  1
END
END UNSATURATED FLOW



VTP    UNSATURATED TRANSPORT MODEL
CONTROL PARAMETERS
***   NLAY      DUMMY      IADU      ISOL        N      NTEL     NGPTS       NIT      DUMMY      DUMMY
         1         20         1         1       18         3       104         2          1          1
***  WTFUN
     1.200


END CONTROL PARAMETERS
TRANSPORT PARAMETER
ARRAY VALUES
***   UNSATURATED TRANSPOR VARIABLES

***            VARIABLE NAME                UNITS               DISTRIBUTION   PARAMETERS            LIMITS
***                                                                              MEAN      STD DEV    MIN       MAX
 ********************************************************************************************************************
 1 Thickness of layer (m)                                          0       6.10      -999.     0.100E-08 -999.
 2 Longit disper of layer (m)                                      0       0.400     -999.     0.000E+00 0.100E+05
 3 Percent organic matter                                          0       0.260E-01 -999.     0.000E+00  100.
 4 Bulk dens of soil layer (g/cc)                                  0        1.45     -999.     0.100E-01  5.00
 5 Biological decay coeff (1/yr)                                   0       0.000E+00 -999.     0.000E+00 -999.
END ARRAY

END LAYER  1
END UNSATURATED TRANSPORT PARAMETERS
END TRANSPORT MODEL
```

(continued)

TABLE 7-8. INPUT SEQUENCE FOR EXAMPLE 3 (concluded).

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
```

```
AQUIFER SPECIFIC VARIABLE DATA
ARRAY VALUES
***       AQUIFER SPECIFIC VARIABLES
```

*** VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
1 Particle diameter (cm)		0	0.630E-03	-999.	0.100E-08	100.
2 Aquifer porosity		-2	-999.	-999.	0.100E-08	0.990
3 Bulk density (g/cc)		-2	-999.	-999.	0.100E-01	5.00
4 Aquifer thickness (m)		0	78.6	-999.	0.100E-08	0.100E+06
5 Mixing zone depth (m)		-1	-999.	-999.	0.100E-08	0.100E+06
6 Hydraulic conductivity (m/yr)		-2	-999.	-999.	0.100E-06	0.100E+09
7 Hydraulic Gradient		0	0.306E-01	-999.	0.100E-07	-999.
8 Grndwater seep velocity (m/yr)		-2	-999.	-999.	0.100E-09	0.100E+09
9 Retardation coefficient		-1	-999.	-999.	1.00	0.100E+09
10 Longitudinal dispersivity (m)		1	160.	15.0	50.0	200.
11 Transverse dispersivity (m)		0	15.2	-999.	0.100E-02	0.100E+05
12 Vertical dispersivity (m)		0	8.00	-999.	0.100E-02	0.100E+05
13 Temperature of aquifer (C)		0	14.4	-999.	0.000E+00	100.
14 pH		4	-999.	-999.	5.80	6.90
15 Organic carbon content (fract)		0	0.315E-02	-999.	0.100E-05	1.00
16 Receptor distance from site(m)		0	152.	-999.	1.00	-999.
17 Angle off center (degree)		0	0.000E+00	-999.	0.000E+00	360.
18 Well vert dist from water tabl		0	0.000E+00	-999.	0.000E+00	1.00

```
END ARRAY

END AQUIFER SPECIFIC VARIABLE DATA


END ALL DATA
```

The type of distribution associated with each parameter is indicated in the "Distribution" column. The number assigned to each of the distribution types is shown in Table A-4. A value of 0 in the "Distribution" column indicates a constant value for the parameter. A value of -1 or -2 indicates that the parameter is derived from other parameters in the code. As Table A-4 indicates, other values are used for Monte Carlo distributions. For example, the saturated hydraulic conductivity for Material 1 in the unsaturated zone has a value of 2 in the "Distribution" column, which indicates that a lognormal probability density distribution has been assigned to the parameter.

7.3.3 Output

The output from MULTIMED is presented in Tables 7-9 through 7-11. Because the General Data Group flag for the level of output from Monte Carlo runs was set to SOME for this example problem (see Section 5.3.2.2), the output consists of the main output file, the STATS.OUT file, and the SAT1.OUT file. The main output file consists of an echo of the input parameters, selected statistical results, and printer plots of frequency and cumulative frequency. The STATS.OUT file contains a summary of the statistical analyses resulting from the Monte Carlo simulations. The cumulative distribution function of well concentrations (i.e., well concentrations in ascending order) is listed in the SAT1.OUT file. This file can be used by the postprocessor, POSTMED, to produce frequency and cumulative frequency plots of higher quality than those found in the main output file. Examples of these plots are shown in Section 4.2.

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
```

U. S. ENVIRONMENTAL PROTECTION AGENCY

EXPOSURE ASSESSMENT

MULTIMEDIA MODEL

VERSION 3.3, DECEMBER 1988

Developed by Phillip Mineart and Atul Salhotra of
Woodward-Clyde Consultants, Oakland, California
In cooperation with:
Hydrogeologic, Inc., Herndon, Virginia,
Geotrans, Inc., Herndon, Virginia,
and
Aqua Terra Consultants, Mountain View, California

```
1
 Run options
 --- -------


 Example 3 input


 Subtitle D application
 Chemical simulated is DEFAULT CHEMICAL


 Option Chosen                          Saturated and unsaturated zone models
 Run was                                MONTE
 Infiltration input by user
 Number of monte carlo simulations       500
 Run was steady-state
 Reject runs if Y coordinate outside plume
 Reject runs if Z coordinate outside plume
 Gaussian source used in saturated zone model
1
1
 UNSATURATED ZONE FLOW MODEL PARAMETERS
 (input parameter description and value)
 NP     - Total number of nodal points                240
 NMAT   - Number of different porous materials          1
 KPROP  - Van Genuchten or Brooks and Corey             1
 IMSHGN - Spatial discretization option                 1
        1
```

(continued)

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.

OPTIONS CHOSEN

Van Genuchten functional coefficients
User defined coordinate system
1

Layer information

LAYER NO.	LAYER THICKNESS	MATERIAL PROPERTY
1	0.00	1

DATA FOR MATERIAL 1

VADOSE ZONE MATERIAL VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Saturated hydraulic conductivity	cm/hr	LOG NORMAL	0.170E-01	0.200E-01	0.100E-03	0.250
Unsaturated zone porosity	--	NORMAL	0.330	0.100	0.200	0.450
Air entry pressure head	m	CONSTANT	0.000E+00	-999.	0.000E+00	-999.
Depth of the unsaturated zone	m	CONSTANT	6.10	-999.	0.100E-08	-999.

DATA FOR MATERIAL 1

VADOSE ZONE FUNCTION VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Residual water content	--	CONSTANT	0.880E-01	-999.	0.100E-08	1.00
Brook and Corey exponent,EN	--	CONSTANT	0.500	-999.	0.000E+00	10.0
ALFA coefficient	1/cm	CONSTANT	0.900E-02	-999.	0.000E+00	1.00
Van Genuchten exponent, ENN	--	CONSTANT	1.23	-999.	1.00	5.00

1

(continued)

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.

UNSATURATED ZONE TRANSPORT MODEL PARAMETERS

NLAY	- Number of different layers used		1
NTSTPS	- Number of time values concentration calc		20
DUMMY	- Not presently used		1
ISOL	- Type of scheme used in unsaturated zone		1
N	- Stehfest terms or number of increments		18
NTEL	- Points in Lagrangian interpolation		3
NGPTS	- Number of Gauss points		104
NIT	- Convolution integral segments		2
IBOUND	- Type of boundary condition		1
ITSGEN	- Time values generated or input		1
TMAX	- Max simulation time	--	0.0
WTFUN	- Weighting factor	--	1.2

OPTIONS CHOSEN

Stehfest numerical inversion algorithm
Nondecaying continuous source
Computer generated times for computing concentrations

1

DATA FOR LAYER 1

VADOSE TRANSPORT VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
Thickness of layer	m	CONSTANT	6.10	-999.	0.100E-08	-999.
Longitudinal dispersivity of layer	m	CONSTANT	0.400	-999.	0.000E+00	0.100E+05
Percent organic matter	--	CONSTANT	0.260E-01	-999.	0.000E+00	100.
Bulk density of soil for layer	g/cc	CONSTANT	1.45	-999.	0.100E-01	5.00
Biological decay coefficient	1/yr	CONSTANT	0.000E+00	-999.	0.000E+00	-999.

1

(continued)

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

CHEMICAL SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS			
LIMITS		MEAN	STD DEV	MIN	MAX	
Solid phase decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Dissolved phase decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Overall chemical decay coefficient	1/yr	DERIVED	0.000E+00	0.000E+00	0.000E+00	0.100E+11
Acid catalyzed hydrolysis rate	1/M-yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Neutral hydrolysis rate constant	1/yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Base catalyzed hydrolysis rate	1/M-yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Reference temperature	C	CONSTANT	25.0	0.000E+00	0.000E+00	100.
Normalized distribution coefficient	ml/g	CONSTANT	140.	0.000E+00	0.000E+00	-999.
Distribution coefficient	--	DERIVED	0.219	0.000E+00	0.000E+00	0.100E+11
Biodegradation coefficient (sat. zone)	1/yr	CONSTANT	0.000E+00	0.000E+00	0.000E+00	-999.
Air diffusion coefficient	cm2/s	CONSTANT	0.000E+00	0.645E-02	0.000E+00	10.0
Reference temperature for air diffusion	C	CONSTANT	0.000E+00	0.000E+00	0.000E+00	100.
Molecular weight	g/M	CONSTANT	-999.	0.000E+00	0.000E+00	-999.
Mole fraction of solute	--	CONSTANT	-999.	0.100E-01	0.100E-08	1.00
Vapor pressure of solute	mm Hg	CONSTANT	-999.	0.230E-01	0.000E+00	100.
Henry`s law constant	atm-m^3/M	CONSTANT	-999.	0.000E+00	0.100E-09	1.00
RFD value for drinking water	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00
ADIF value for fish consumption	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00
CCC for aquatic organisms	mg-kg/day	CONSTANT	1.00	0.000E+00	0.000E+00	1.00

1

SOURCE SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Infiltration rate	m/yr	CONSTANT	0.700E-02	-999.	0.100E-09	0.100E+11
Area of waste disposal unit	m^2	CONSTANT	400.	-999.	0.100E-01	-999.
Duration of pulse	yr	CONSTANT	-999.	-999.	0.100E-08	-999.
Spread of contaminant source	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Recharge rate	m/yr	CONSTANT	0.160E-01	-999.	0.100E-09	0.100E+11
Source decay constant	1/yr	CONSTANT	0.000E+00	-999.	0.000E+00	-999.
Initial concentration at landfill	mg/l	CONSTANT	1.00	-999.	0.000E+00	-999.
Length scale of facility	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Width scale of facility	m	DERIVED	-999.	-999.	0.100E-08	0.100E+11
Near field dilution		CONSTANT	0.000E+00	0.000E+00	0.000E+00	0.000E+00

1

(continued)

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

AQUIFER SPECIFIC VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
Particle diameter	cm	CONSTANT	0.630E-03	-999.	0.100E-08	100.
Aquifer porosity	--	DERIVED	-999.	-999.	0.100E-08	0.990
Bulk density	g/cc	DERIVED	-999.	-999.	0.100E-01	5.00
Aquifer thickness	m	CONSTANT	78.6	-999.	0.100E-08	0.100E+06
Source thickness (mixing zone depth)	m	DERIVED	-999.	-999.	0.100E-08	0.100E+06
Conductivity (hydraulic)	m/yr	DERIVED	-999.	-999.	0.100E-06	0.100E+09
Gradient (hydraulic)		CONSTANT	0.306E-01	-999.	0.100E-07	-999.
Groundwater seepage velocity	m/yr	DERIVED	-999.	-999.	0.100E-09	0.100E+09
Retardation coefficient	--	DERIVED	-999.	-999.	1.00	0.100E+09
Longitudinal dispersivity	m	NORMAL	160.	15.0	50.0	200.
Transverse dispersivity	m	CONSTANT	15.2	-999.	0.100E-02	0.100E+05
Vertical dispersivity	m	CONSTANT	8.00	-999.	0.100E-02	0.100E+05
Temperature of aquifer	C	CONSTANT	14.4	-999.	0.000E+00	100.
pH	--	UNIFORM	-999.	-999.	5.80	6.90
Organic carbon content (fraction)		CONSTANT	0.315E-02	-999.	0.100E-05	1.00
Well distance from site	m	CONSTANT	152.	-999.	1.00	-999.
Angle off center	degree	CONSTANT	0.000E+00	-999.	0.000E+00	360.
Well vertical distance	m	CONSTANT	0.000E+00	-999.	0.000E+00	1.00

1 0 Values generated which exceeded the specified bounds.
1 ----- RESULTS -----

SATURATED ZONE TRANSPORT

Example 3 input

Subtitle D application

90. PERCENT CONFIDENCE INTERVAL

N	= 500		
MEAN	= 0.573E-03		
STANDARD DEVIATION	= 0.346E-04		
COEFFICIENT OF VARIATION	= 0.604E-01		
MINIMUM VALUE	= 0.475E-03		
MAXIMUM VALUE	= 0.657E-03		
50th PERCENTILE	= 0.573E-03	0.570E-03	0.576E-03
80th PERCENTILE	= 0.602E-03	0.599E-03	0.605E-03
85th PERCENTILE	= 0.608E-03	0.605E-03	0.614E-03
90th PERCENTILE	= 0.619E-03	0.614E-03	0.623E-03
95th PERCENTILE	= 0.634E-03	0.626E-03	0.640E-03

(continued)

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.
44444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

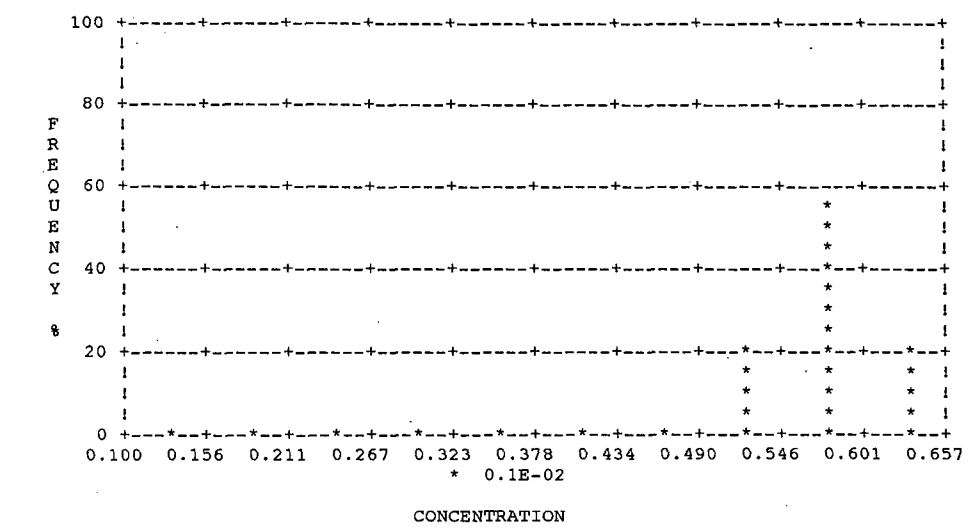
-999 UNABLE TO COMPUTE CONFIDENCE BOUND DUE TO INSUFFICIENT DATA

VALUE	% OF TIME EQUALLED OR EXCEEDED	% OF TIME IN INTERVAL
0.100E-03	100.000	
		0.000
0.156E-03	100.000	
		0.000
0.211E-03	100.000	
		0.000
0.267E-03	100.000	
		0.000
0.323E-03	100.000	
		0.000
0.378E-03	100.000	
		0.000
0.434E-03	100.000	
		0.800
0.490E-03	99.200	
		21.400
0.546E-03	77.800	
		56.800
0.601E-03	21.000	
		20.800
0.657E-03	0.200	

1

(continued)

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.



(continued)

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

1
 C 100 +------+------+------+------+------+------+------+------+------+-----**
 U     !                                                             *** !
 M     !                                                          *    !
 U     !                                                       *       !
 L  80 +------+------+------+------+------+------+------+------+------*------+
 A     !                                                             .  !
 T     !                                                          *     !
 I     !                                                       *        !
 V  60 +------+------+------+------+------+------+------+------+------+------+
 E     !                                                    *           !
       !                                                                !
 F     !                                                 *              !
 R  40 +------+------+------+------+------+------+------+------+-*----+------+
 E     !                                                 .              !
 Q     !                                              *                 !
 U     !                                                                !
 E  20 +------+------+------+------+------+------+------+------*------+------+
 N     !                                                    *           !
 C     !                                                 *              !
 Y     !                                              **                !
    0 +**************************************************----+------+------+
   0.100  0.156  0.211  0.267  0.323  0.378  0.434  0.490  0.546  0.601  0.657
                                 *  0.1E-02

                                CONCENTRATION
```

(continued)

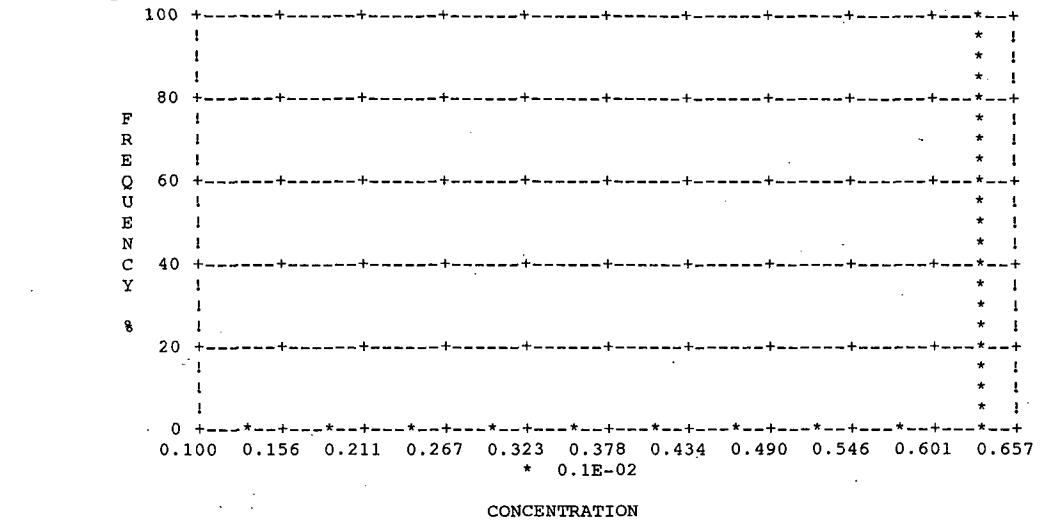
TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3.

```
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

1

 FOLLOWING GRAPHS ARE FOR THE TOP 20% OF THERESULTS
1
   100 +------+------+------+------+------+------+------+------+------+---*--+
       !                                                                *  !
       !                                                                *  !
       !                                                                *  !
    80 +------+------+------+------+------+------+------+------+------+---*--+
 F     !                                                                *  !
 R     !                                                                *  !
 E     !                                                                *  !
 Q  60 +------+------+------+------+------+------+------+------+------+---*--+
 U     !                                                                *  !
 E     !                                                                *  !
 N     !                                                                *  !
 C  40 +------+------+------+------+------+------+------+------+------+---*--+
 Y     !                                                                *  !
       !                                                                *  !
 %     !                                                                *  !
    20 +------+------+------+------+------+------+------+------+------+---*--+
       !                                                                *  !
       !                                                                *  !
       !                                                                *  !
     0 +---*--+---*--+---*--+---*--+---*--+---*--+---*--+---*--+---*--+---*--+
    0.100  0.156  0.211  0.267  0.323  0.378  0.434  0.490  0.546  0.601  0.657
                                  *  0.1E-02

                                CONCENTRATION
```



(continued)

TABLE 7-9. MAIN OUTPUT FILE FOR EXAMPLE 3 (concluded).

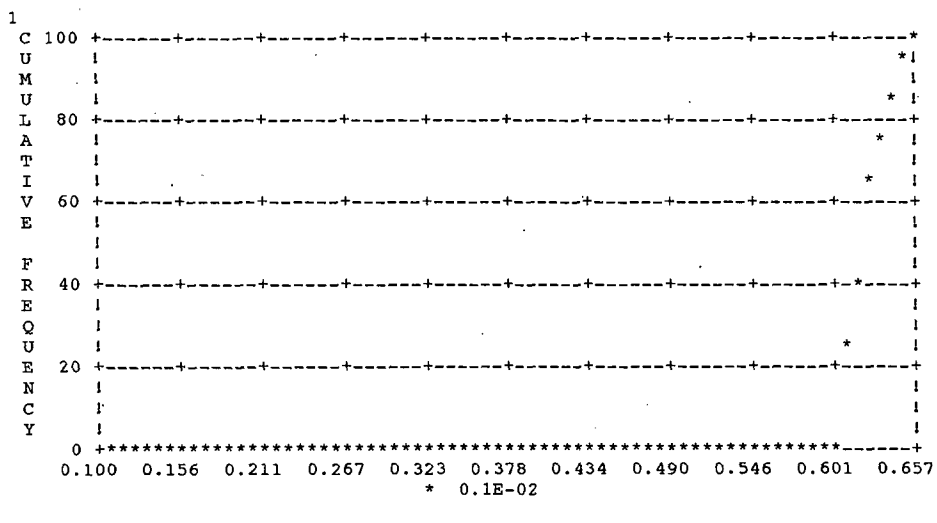


TABLE 7-10. FIRST PAGE OF THE SAT1.OUT FILE FOR EXAMPLE 3.
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

```
0.47457E-03
0.47974E-03
0.48608E-03
0.48800E-03
0.49012E-03
0.49224E-03
0.49897E-03
0.49929E-03
0.49976E-03
0.50186E-03
0.50328E-03
0.50413E-03
0.50599E-03
0.50715E-03
0.50830E-03
0.50845E-03
0.50892E-03
0.50896E-03
0.50899E-03
0.50927E-03
0.50953E-03
0.51086E-03
0.51110E-03
0.51265E-03
0.51344E-03
0.51375E-03
0.51534E-03
0.51589E-03
0.51801E-03
0.51807E-03
0.51846E-03
0.52211E-03
0.52246E-03
0.52261E-03
0.52275E-03
0.52347E-03
0.52361E-03
0.52425E-03
0.52430E-03
0.52450E-03
0.52490E-03
0.52494E-03
0.52552E-03
0.52583E-03
0.52599E-03
0.52603E-03
0.52615E-03
0.52751E-03
```

TABLE 7-11. STATS.OUT FILE FOR EXAMPLE 3.

4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

1 ----- RESULTS -----

SATURATED ZONE TRANSPORT

Example 3 input

Subtitle D application

			90. PERCENT CONFIDENCE INTERVAL	
N	=	500		
MEAN	=	0.573E-03		
STANDARD DEVIATION	=	0.346E-04		
COEFFICIENT OF VARIATION	=	0.604E-01		
MINIMUM VALUE	=	0.475E-03		
MAXIMUM VALUE	=	0.657E-03		
50th PERCENTILE	=	0.573E-03	0.570E-03	0.576E-03
80th PERCENTILE	=	0.602E-03	0.599E-03	0.605E-03
85th PERCENTILE	=	0.608E-03	0.605E-03	0.614E-03
90th PERCENTILE	=	0.619E-03	0.614E-03	0.623E-03
95th PERCENTILE	=	0.634E-03	0.626E-03	0.640E-03

-999 UNABLE TO COMPUTE CONFIDENCE BOUND DUE TO INSUFFICIENT DATA

VALUE	% OF TIME EQUALLED OR EXCEEDED	% OF TIME IN INTERVAL
0.100E-03	100.000	
		0.000
0.156E-03	100.000	
		0.000
0.211E-03	100.000	
		0.000
0.267E-03	100.000	
		0.000
0.323E-03	100.000	
		0.000
0.378E-03	100.000	
		0.000
0.434E-03	100.000	
		0.800
0.490E-03	99.200	
		21.400
0.546E-03	77.800	
		56.800
0.601E-03	21.000	
		20.800
0.657E-03	0.200	

APPENDIX A

CODE STRUCTURE AND INPUT DATA FORMAT

MULTIMED consists of a number of modules, the theoretical details of which are described in Salhotra et al. (1990). It is important for the user to understand the capabilities and limitations of these modules. However, because an interactive preprocessor, PREMED, has been developed to create or edit input, the average user need not understand the format of the input files or the structure of the code. For advanced users, who wish to modify the code or to examine the input files without the use of the preprocessor, this chapter provides an overview of the code structure and input file format. Much of the information in this appendix is based on material in Salhotra and Mineart (1988). No information about the pre- and postprocessors for MULTIMED is included.

A.1 MODEL STRUCTURE

The code consists of a number of subroutines. The organization of the subroutines is shown in Figure A.1. In addition, a list of all the subroutines, the calling subroutine/program, and a brief description of the subroutines is included in Appendix B. Each subroutine includes several comment statements that describe the function of the subroutine. The arguments of each subroutine are divided into three categories: 1) arguments that are passed to the subroutine by the calling program, 2) arguments that are modified within the subroutine, and 3) arguments returned by the subroutine to the calling program.

A.2 INPUT AND OUTPUT FILE UNITS

To run the model, one or two input files are needed, depending on the options selected by the user. The location of the open statements for these files, the default unit numbers, file names, and contents are shown in Table A-1.

The model generates a number of output files. The location of the open statements for these files, the associated default unit numbers, file names, and a brief description are given in Table A-2.

The user specifies the name of the main output file. In deterministic mode, this file contains an echo of the input data and the calculated contaminant concentration(s) at the receptor(s) of interest. In Monte Carlo mode, the file consists of an echo of input parameters, selected statistical results, and printer plots of frequency and cumulative frequency.

Two additional types of files are also generated. These are designated as the *.VAR and *.OUT files, where the "*" refers to a specific type of data for the

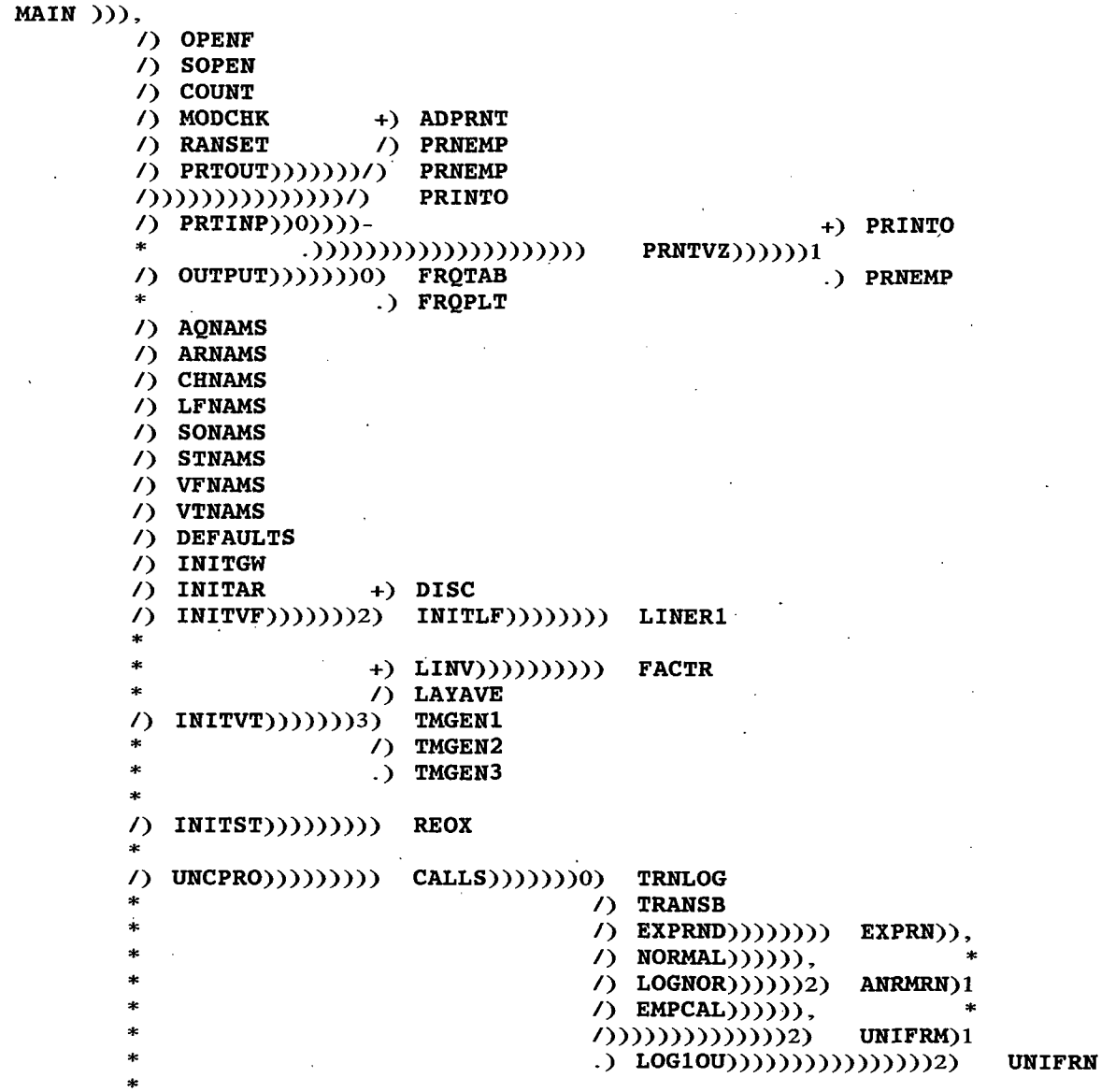


Figure A.1 Subroutine organization tree for MULTIMED (from Salhotra and Mineart, 1988).

(continued)

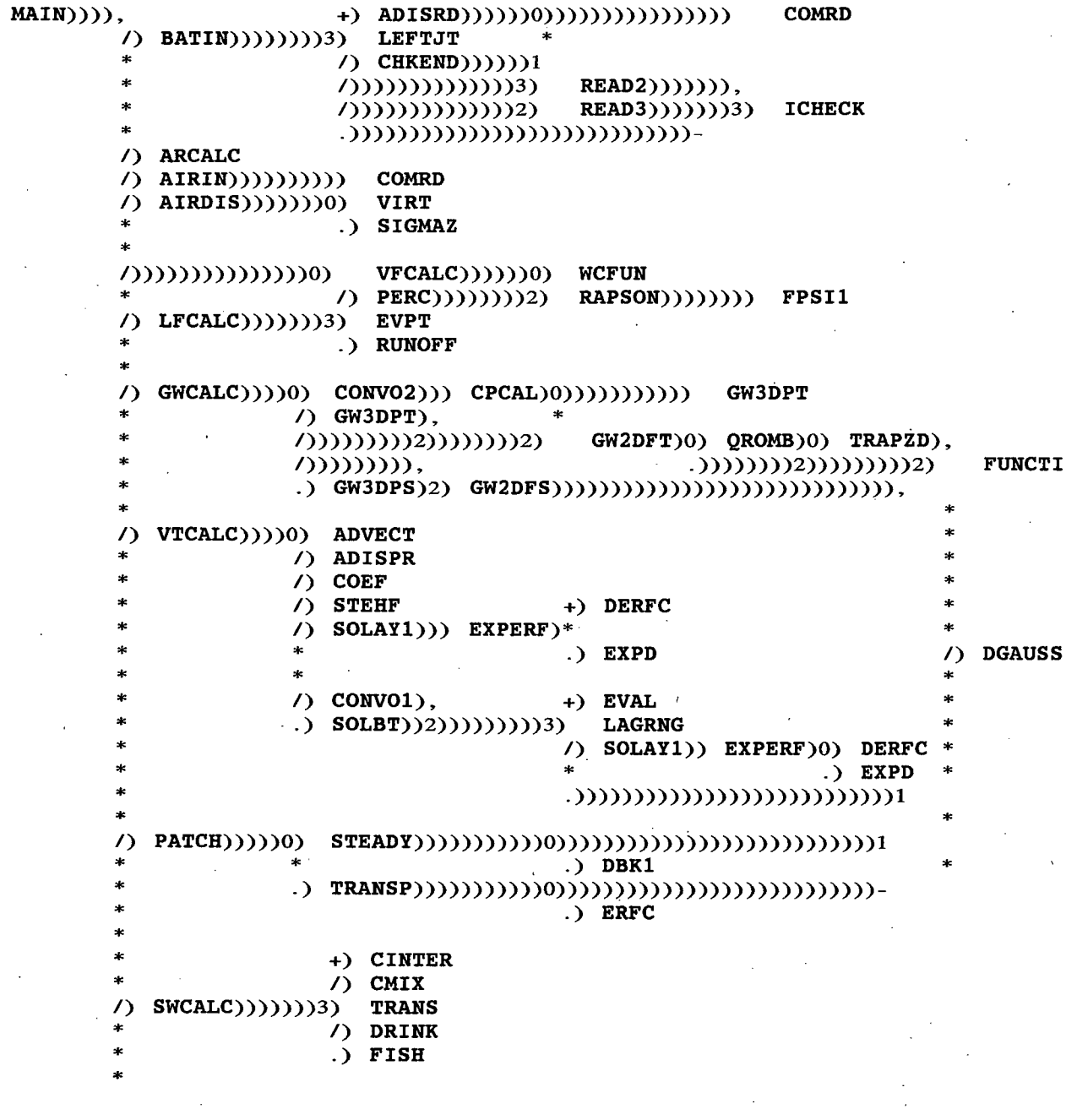


Figure A.1 Subroutine organization tree for MULTIMED (from Salhotra and Mineart, 1988). (concluded)

Table A-1. INPUT FILES NEEDED IN MULTIMED

Opened In	Unit	Name	Description
MAIN	IOUT7=7	USER-SPECIFIED	Main input file. Required to run the model.
ADISRD	IUNT28=28	FREQ.IN	Contains information describing the wind-stability joint frequency distribution for contaminant transport in the air (see Section A.5.9.1).

.VAR files and a specific module for the .OUT files. The *.VAR files contain the values of the randomly-generated variables, any derived variables used for each Monte Carlo simulation run, and the values of any deterministic variables. The .OUT files contain the model results for each Monte Carlo simulation. Thus, for typical Monte Carlo simulations, these files will contain 500 to 2000 values. Results of statistical analyses (mean, median, and percentiles) of the values in the *.OUT files are included in the main output file and in the file STATS.OUT.

The BATCH.ECH file contains an echo of all the data in the input file and includes any error messages generated while reading the data. Errors in reading the data will stop execution of the program.

Two of the output files may be used with the postprocessor, POSTMED. The data in SAT1.OUT can be used by the postprocessor to generate frequency and cumulative frequency plots. For transient, deterministic simulations, plots of concentration versus time can be generated by the postprocessor using data in the main input file.

A.3 COMMON BLOCKS AND PARAMETER STATEMENTS

Most variables are passed between subroutines through the use of common blocks. There are a total of 54 common blocks in the model (i.e., excluding those associated with the pre- and postprocessors), each containing a related set of variables. The common blocks are contained in files which are accessed by the code during compilation through the use of INCLUDE statements located at the beginning of each subroutine.

Parameter statements are used to define all I/O (Input/Output) unit numbers and array dimensions in the model. Any array dimensions or I/O numbers can be changed by assigning a new value to the variable in the appropriate parameter statement. The entire code must be recompiled and linked if changes are made to any parameter statement.

TABLE A-2. OUTPUT FILES GENERATED BY MULTIMED

Opened In	Unit	Name	Description
MAIN	IOUT = 1	user-specified	Main output file.
SOPEN	IUNT8 = 8	AQUIFER.VAR	Values of aquifer variables generated for Monte Carlo simulations.
SOPEN	IUNT13 = 13	CHEMICAL.VAR	Values of chemical variables generated for Monte Carlo simulations.
SOPEN	IUNT14 = 14	SOURCE.VAR	Values of source variables generated for Monte Carlo simulations.
SOPEN	IUNT15 = 15	SURFACE.VAR	Values of surface water variables generated for Monte Carlo simulations.
SOPEN	IUNT16 = 16	VFLOW.VAR	Values of unsaturated zone material variables and functional parameters generated for Monte Carlo simulations.
SOPEN	IUNT17 = 17	VTRNSPT.VAR	Values of unsaturated zone transport variables generated for Monte Carlo simulations.
SOPEN	IUNT18 = 18	AIR.VAR	Values of Air Emissions and Dispersion Module variables generated for Monte Carlo simulations.
BATIN	BATOUT = 19	BATCH.ECH	Echo of the batch input file and list of any errors in the input data.
SOPEN	VFOUT = 20	VFLOW.OUT	Results from the Unsaturated Zone Flow Module.
SOPEN	VTOUT = 21	VTRNSPT.OUT	Concentrations at the water table computed by the Unsaturated Zone Transport Module.

(continued)

TABLE A-2. OUTPUT FILES GENERATED BY MULTIMED (concluded)

Opened In	Unit	Name	Description
SOPEN	STOUT = 22	SAT.OUT	Downgradient well concentrations computed by Saturated Zone Transport Module.
SOPEN	AROUT = 23	AIR.OUT	Results from Air Emissions Module and the receptor concentrations for the Air Dispersion Module.
SOPEN	STOUT2 = 24	SURFACE.OUT	Results from the Surface Water Module.
MAIN	ISTAT = 25	STATS.OUT	Summary statistics of the receptor concentrations (groundwater, atmosphere, surface stream).
MAIN	IUNT27 = 27	SAT1.OUT	Downgradient well concentrations sorted in ascending order (CDF of concentrations).
SOPEN	IUNT29 = 29	LANDFM.VAR	Values of landfill material parameters generated for Monte Carlo simulations.
SOPEN	IUNT30 = 30	LANDFL.VAR	Values of liner properties generated for Monte Carlo simulations.
SOPEN	IUNT31 = 31	LANDFH.VAR	Values of hydrology parameters generated for Monte Carlo simulations.

The main output contains an echo of the input data, printer plots, and selected statistical parameters of the results of the Monte Carlo simulations. In addition, a summary output file is created on unit ISTAT.

A.4 STRUCTURE OF THE INPUT FILES

The overall structure of the main input file is shown in Figure A.2. The first two cards contain the title of the simulation. The remaining cards in the file contain the data necessary to run MULTIMED. These data are clustered into a number of groups, each of which contains a specific type of data that is input using one or more DATA CARDS. The data groups are divided into subgroups, with each subgroup containing a set of data specific to the group within which the subgroup is located. The structure of each data group/subgroup is illustrated in Figure A.2. In addition to the DATA CARDS, the input file contains DATA GROUP/SUBGROUP SPECIFICATION CARDS, END CARDS, and if desired, one or more COMMENT CARDS.

The data for the model are divided into nine major groups. These groups are listed in Table A-3 along with the appropriate code for the GROUP SPECIFICATION CARD. Each data group is read in as a unit, with the beginning identified by the GROUP SPECIFICATION CARD and the end by the END CARD. The data cards are sandwiched between these two cards. Further, the data group may contain one or more subgroups that are also listed in Table A-3. Note that the structure of a subgroup is exactly the same as that for a group--i.e., a subgroup is identified by a SUBGROUP SPECIFICATION CARD and terminated by an END CARD, with the subgroup data sandwiched between the two cards. A data file need contain only those data groups (and subgroups within a data group) that are necessary to run the options selected by the user.

The options selected by the user and indicated in the General Data Group will determine which additional groups of data are necessary. For example, if the user has specified within the General Data Group that only the Saturated Zone Transport Module will be run, the Unsaturated Zone Flow and Transport Data Groups (VFL, VTP) are not necessary. Also note that the structure of the input file allows the required data groups to be arranged in any order.

A.4.1 Comment Cards

COMMENT CARDS are indicated by the presence of three asterisks, '***'. The group of '***' can be input starting at any column of the card but must be the first three non-blank characters. The COMMENT CARDS are useful for separating data types and can be used to include other helpful comments. Note that there are no restrictions as to the location and number of COMMENT CARDS, except that they cannot be the first two cards in the data file.

A.4.2 Data Group/Subgroup Specification Card, End Card, and Data Cards

The DATA GROUP/SUBGROUP SPECIFICATION CARD indicates the beginning of a specific data group and includes the Group (Subgroup) Specification Code (Table A-3) in columns 1 to 3. For example, if the DATA GROUP SPECIFICATION CARD contains the letters 'AQU' in columns 1 to 3, it implies that the following cards, up to and including the corresponding 'END' card, contain aquifer data.

With the exceptions discussed in Section A.5, each DATA CARD contains information about one variable only. Typically the card will contain the variable

Figure A.2

Table A-3. INPUT DATA GROUPS AND SUBGROUPS IN MULTIMED

Data Group	Group Specification Code
1. General Data	GEN
2. Source Data	SOU
3. Landfill Data	LFL
4. Chemical Data	CHE
5. Unsaturated Zone Flow Data	VFL
6. Unsaturated Zone Transport Data	VTP
7. Aquifer Data	AQU
8. Surface Water Data	SUR
9. Air Emissions and Dispersion Data	AIR

Subgroups	Subgroup Specification Code
1. Array Data	ARR
2. Empirical Distribution Data	EMP
3. Control Data	CON
4. Spatial Discretization Data	SPA
5. Material Property Data	SAT
6. Material Specification Data	MAT
7. Unsaturated Zone Moisture Data	SOI
8. Unsaturated Zone Transport Properties Data	TRA
9. Unsaturated Zone Time Stepping Data	TIM
10. Landfill Liner Data	LIN
11. Layer Identification Data	LAY
12. Hydrology Data	HYD

specification index, variable name, Monte Carlo distribution type, distribution parameters, and the upper and lower bounds of the distribution. To the extent possible, consistent formats for the DATA CARDS have been maintained for the different data groups.

The termination of a data group and/or a subgroup is indicated by the END CARD, which contains the word END in the first three columns.

A.4.3 Specification of Parameter Values

Within each group, except the General Data Group, there are a number of variables whose value can be specified in one of three ways: 1) the variable may be assigned a constant value, 2) the variable may be derived within the code using functional relations--for example, the aquifer porosity may be derived from the particle diameter, or 3) the variable may be assigned a distribution and the value randomly generated in the Monte Carlo simulation. The numerical codes associated with each distribution type are listed in Table A-4. Depending on

Table A-4. DISTRIBUTIONS AVAILABLE AND THEIR CODES

Distribution Type	Distribution Code
Constant	0
Normal	1
Lognormal	2
Exponential	3
Uniform	4
Log10 Uniform	5
Empirical	6
Johnson SB	7
Gelhar[a]	8
Derived Dispersivity[b]	10
Derived Variable[c]	-1

[a] Gelhar's distribution applies only to the saturated zone dispersivities. For details, refer to Section 6.5.10.

[b] The derivation of the saturated zone dispersivities using distribution code 8 is described in Section 5.5.3.5 of Salhotra et al. (1990).

[c] For parameters other than the spread of the source or the source thickness (mixing zone depth), a -2 is interchangeable with a -1.

Note: The seven Monte Carlo distributions (distribution code 1-7) are described in Section 9.4 of Salhotra et al. (1990).

the distribution selected for a particular variable, the required input data will vary. Refer to Section 9.4 of Salhotra et al. (1990) for information about the seven Monte Carlo distribution options. Section 5.5.3.5 of Salhotra et al. (1990) or Section 6.5.10 of this document explain the Gelhar distribution and the derivation of dispersivity.

A.4.4 The Array Subgroup

The contents and format for the Array Subgroup are shown in Table A-5. The first card is the SUBGROUP SPECIFICATION CARD, with the code ARR in the first three columns. This card is followed by one card for each variable in the group. Those cards contain values/distributions, and lower and upper bounds for the indicated variables. For example, when the ARR subgroup is included within the Aquifer Group Data, the subgroup will contain cards describing the aquifer-specific variables such as porosity, dispersivities, etc. The specific variables within each group are discussed in Section A.5. Note that the number of cards within the Array Subgroup varies because the various groups and subgroups have different numbers of input variables. The variable being input is identified by the value of the Index I.

Table A-5. CONTENTS AND FORMAT OF A TYPICAL ARRAY SUBGROUP

Card	Contents	Format
A1	"ARR"	A3
A2	I, NAME(I), NDSTPRM(I), ARRPRM(I,1) ARRPRM(I,2), BOUND(I,1), BOUND(I,2)	I2, 1X, A50, 7X, I10, 5X, 4F10.0
A3	"END"	A3

Note: Card/line A2 is repeated for each variable within the group.

Definition of Contents

"ARR" Subgroup Specification Card indicating the start of the Array Subgroup.

I Integer which identifies the variable being input. See the individual data group tables for the values of I for specific variables. Note that I is not a counter.

NAME(I) Name of variable I. It is used to identify the variables in the output files.

NDSTPRM(I) Integer which identifies the type of distribution used for variable I (e.g., constant, derived, or one of the Monte Carlo distributions). See Table A-4.

ARRPRM(I,1) Mean value for variable I.

ARRPRM(I,2) Standard deviation for variable I.

BOUND(I,1) Minimum allowed value (lower bound) for variable I.

BOUND(I,2) Maximum allowed value (upper bound) for variable I.

"END" End Card indicating the end of the Array Subgroup.

The value of the integer variable NDSTPRM(I) in Table A-5 indicates the type of distribution chosen for the variable identified by the index I. The available options and values of the integer variable NDSTPRM(I) are listed in Table A-4. If any of the variables are specified to have an Empirical distribution (NDSTPRM(I) = 6), then it is necessary to include the EMPIRICAL SUBGROUP, the details of which are described in Section A.4.5. Note that if the variable is specified to be a constant (NDSTPRM(I) = 0), the value input as mean for the corresponding variable (ARRPRM(I,1)) is used in the simulations. The end of the Array Subgroup is indicated by an END CARD.

A.4.5 The Empirical Distribution Subgroup

The contents and format for the Empirical Distribution Subgroup are shown in Table A-6. The first card is the SUBGROUP SPECIFICATION CARD, with the code EMP in the first three columns. The next card identifies the variable (using the index I) that has an empirical distribution and the number of coordinates of the empirical cumulative distribution function that are being input. A maximum of 20 coordinates can be input.

The next set of cards (two cards, if fewer than 10 coordinate pairs are input, or four cards, if more than 10 coordinate pairs are input) contain the probabilities

(in ascending order) and the corresponding values of the variable. Variable values corresponding to cumulative probability values of zero and unity must be provided. Note that all the cumulative probability coordinate values are first input, followed by an equal number of the corresponding variable values. The above procedure is repeated for each of the variables that have empirical distributions. The end of the subgroup is indicated by the END CARD.

A.5 FORMAT OF THE DATA GROUPS

As was stated above, DATA CARDS 1 and 2 contain the title of the run, with a maximum of 80 columns per card. DATA CARDS 3 through the end contain data specific to one or more groups/subgroups. The specific formats for each data group are described below. The data groups do not have to be input in the order in which they are discussed. However, it is recommended that the General Data Group be input first. An END CARD must be put at the end of the data file following the end of the last data group.

A.5.1 General Data Group

The contents and format of the General Data Group are shown in Table A-7. This group can contain up to six cards. The first card is the GROUP SPECIFICATION CARD and has the code GEN in the first three columns. The second card contains the name of the chemical being simulated. Card three contains a number of variables that enable the user to select the model options. A schematic showing key options pertaining to the Saturated Zone Module is indicated in Figure A.3. If transport in a stream (Surface Water Module) is simulated, the variable XST is the fourth card and indicates the distance from the point of groundwater plume interception to the water supply intake. The next card, i.e. values of TPSTN(I), is necessary only if the Saturated Zone Module is run in the unsteady state and contains the time values at which the saturated zone results are to be computed. The final card is the END CARD that indicates the termination of this set of data. Table A-8 is an example of a typical General Data Group.

A.5.2 Source Data Group

The contents and format for the Source Data Group are shown in Table A-9. This group describes the contaminant source-specific data. The first card is the

Table A-6. CONTENTS AND FORMAT OF A TYPICAL EMPIRICAL DISTRIBUTION SUBGROUP

Card	Contents	Format
E1	"EMP"	A3
E2	I, ICOUNT	2I10
E3	EMPPRM(J,2,I), J= 1,ICOUNT	10(F8.0, 2X)
E4	EMPPRM(J,1,I), J= 1,ICOUNT	10(F8.0, 2X)
E5	"END"	A3

Note: Card/lines E3 and E4 are repeated twice if more than 10 coordinates are input. Card/lines E2, E3, and E4 are repeated if more than one variable has an empirical distribution.

Definition of Contents

"EMP"	Subgroup Specification Card indicating the start of the Empirical Distribution Subgroup.
I	Integer which identifies the variable being input. See the individual data group tables for the values of I for specific variables. Note that I is not a counter.
ICOUNT	Number of coordinates of the empirical cumulative frequency distribution.
EMPPRM(J,2,I)	Cumulative probability (coordinate) values for the empirical distribution for variable I.
EMPPRM(J,1,I)	Corresponding variable values associated with the above probabilities.
"END"	End Card indicating the end of the Empirical Distribution Subgroup.

Table A-7. CONTENTS AND FORMAT OF THE GENERAL DATA GROUP

Card	Contents	Format
G1	"GEN"	A3
G2	CHEMICAL	80A1
G3	OPTION, ISOURC, OPTAIR, RUN, MONTE, ROUTE, ISTEAD, NT, IOPEN, IYCHK, IZCHK PALPH, LANDF, APPTYP, COMPLETE	3I5, 5X, A13, 2X, 7I5, F5.0, 3I5
G4	XST	F10.0
G5	TPSTN(I), I = 1, NT	10(F8.0, 2X)
G6	"END"	A3

Definition of Contents

"GEN" Group Specification Card indicating the start of the General Data Group.

CHEMICAL Name of chemical being simulated.

OPTION Integers defining which scenario to run.

1	Saturated Zone Transport Module only
2	Unsaturated and Saturated Zone Modules
3	Unsaturated, Saturated and Surface Water Modules
4	Saturated Zone and Surface Water Modules
6	Air Modules only

ISOURC Flag indicating the type of saturated zone boundary condition.

0	Gaussian source
1	Patch source

OPTAIR Flag indication which air modules to run.

0	No air modules are run
1	Air Emissions Module run
2	Air Emissions and Air Dispersion Modules run

RUN Flag indicating the type of run.
DETERMINISTIC
MONTE

MONTE The number of Monte Carlo simulations to be performed.

Table A-7. CONTENTS AND FORMAT OF THE GENERAL DATA GROUP (continued)

		Definition of Contents
ROUTE		Flag indicating the exposure route for the Surface Water Module. (This parameter is ignored if not running the Surface Water Module.)
	1	Human exposure through drinking water
	2	Human exposure through fish consumption
	3	Exposure to aquatic organisms
ISTEAD		Flag indicating unsteady- or steady-state simulation of the unsaturated and saturated zone transport.
	0	Unsteady-state
	1	Steady-state
NT		Number of time steps for which unsteady-state saturated zone transport results are required.
IOPEN		Integer flag indicating the information to be output.
	0	Opens all *.VAR and *.OUT files
	1	Opens only the main output file, STATS.OUT, and SAT1.OUT
	2	Opens only the main output file and STATS.OUT
XST		Instream distance between the point of groundwater loading to the downstream water supply intake. Include only when running the Surface Water Module.
TPSTN(I)		Times at which unsteady-state transport results for the saturated zone are required (Needed only when ISTEAD = 0).
IYCHK		Flag for rejecting well locations outside of the groundwater plume width when in Monte Carlo mode.
	0	Rejects the generated receptor well location y-coordinate value
	1	Does not reject the generated y-coordinate value
IZCHK		Flag for rejecting well locations outside of the groundwater plume depth when in Monte Carlo mode.
	0	Rejects the generated receptor well location z-coordinate value
	1	Does not reject the generated z-coordinate value
PALPH		The selected confidence level, in percent, for the four estimated percentiles (80th, 85th, 90th, 95th).
LANDF		Flag for running the Landfill Module.
	0	Do not run the Landfill Module
	1	Run the Landfill Module

Table A-7. CONTENTS AND FORMAT OF THE GENERAL DATA GROUP (concluded)

Definition of Contents	
APPTYP	Flag for the type of application being simulated.
1	Generic MULTIMED application
2	Subtitle D MULTIMED application
COMPLETE	Flag indicating whether all the necessary input parameters have been defined (parameter used in the preprocessor).
0	Undefined parameters exist in the input
1	No undefined parameters exist in the input
"END"	End Card indicating the end of the General Data Subgroup.

GROUP SPECIFICATION CARD, with the code SOU in the first three columns. This is followed by the Array Subgroup, which is indicated by the SUBGROUP SPECIFICATION CARD with the code ARR in the first three columns. Details of the Array Subgroup were presented in Table A-5 and Section A.4.4. This subgroup contains an array of information about the values and/or the distributions and lower and upper bounds of (up to) nine source-specific variables. The variables associated with each index I are listed in Table A-10.

If any of the variables are specified to have an empirical distribution (NDSTPRM(I) = 6), then it is necessary to include the Empirical Distribution Subgroup discussed in Section A.4.5. If none of the source-specific variables have an empirical distribution, this subgroup is not necessary.

Of the nine variables included in this group, three can be derived. These are the spread of input source, the length scale, and the width scale of the facility. Thus, NDSTPRM(4), NDSTPRM(8), and NDSTPRM(9) can have values less than zero (see Table A-4). The methods used to derive these variables are discussed in Section 5.5.1 of Salhotra et al. (1990) or Section 6.2 of this manual.

Note that if the user specifies LANDF=1 in the General Data Group (i.e., uses the Landfill Module to compute infiltration) the value of infiltration specified in the Source Data Group (Table A-10) is ignored.

An END CARD indicates the end of the Source Data Group.

A.5.3 Landfill Data Group

This group contains data required by the Landfill Module and consists of four subgroups. It is required only if the infiltration is not input by the user in the Source Data Group. The subgroups and the associated codes are listed below:

Figure A.3

TABLE . .. EXAMPLE OF A TYPICAL GENERAL DATA GROUP

```
GENERAL DATA

***  CHEMICAL NAME FORMAT(80A1)
DEFAULT CHEMICAL

***     ISOURC                                ROUTE       NT        IYCHK    PALPH       APPTYP
***OPTION    OPTAIR  RUN              MONTE     ISTEAD      IOPEN       IZCHK      LANDF    COMPLETE
    3     0     0     DETERMINISTIC    500     1     1     1     0     0     1 90.0     1     1     0


***XST
   1000.00

END GENERAL
```

Table A-9. CONTENTS AND FORMAT OF THE SOURCE-SPECIFIC DATA GROUP

Card	Contents	Format
S1	"SOU"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
S2	"END"	A3

Definition of Contents

"SOU"	Group Specification Card indicating the start of the Source Data Group.
Array Subgroup	Subgroup defining the source variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of the Source Data Group.

Subgroup	Specification Code	Refer to Table
Control Data	CON	A-11
Layer Thickness and Material Data	LAY	A-12
Liner Property Data	LIN	A-13
Landfill Material Property Data	SAT	A-15
Hydrologic Data	HYD	A-17

The first card of this group is the GROUP SPECIFICATION CARD and includes the code LFL in the first three columns. The next card is the first subgroup specification card and includes the appropriate code shown above. Data for each of the subgroups of the Landfill Module are described below. None of the variables in this group can be derived (i.e., they cannot have a distribution type of -1).

Note that some of the input units for the Landfill Module are non-metric. These data are automatically converted from the input units to the metric system of units by the code before computations are performed.

TABLE A-10. VARIABLES IN THE SOURCE-SPECIFIC ARRAY SUBGROUP

SOURCE SPECIFIC VARIABLE DATA
ARRAY VALUES
*** SOURCE SPECIFIC VARIABLES

*** VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
1 Infiltration rate	(m/yr)	0	-999.	-999.	0.100E-09	0.100E+11
2 Area of waste disp unit	(m^2)	0	-999.	-999.	0.100E-01	-999.
3 Duration of pulse	(yr)	0	-999.	-999.	0.100E-08	-999.
4 Spread of contaminant srce	(m)	-1	-999.	-999.	0.100E-08	0.100E+11
5 Recharge rate	(m/yr)	0	-999.	-999.	0.100E-09	0.100E+11
6 Source decay constant	(1/yr)	0	-999.	-999.	0.000E+00	-999.
7 Init conc at landfill	(mg/l)	0	1.00	-999.	0.000E+00	-999.
8 Length scale of facility	(m)	-1	-999.	-999.	0.100E-08	0.100E+11
9 Width scale of facility	(m)	-1	-999.	-999.	0.100E-08	0.100E+11

END ARRAY

END SOURCE SPECIFIC VARIABLE DATA

A.5.3.1 Landfill Control Data Subgroup--

Table A-11 describes the landfill control subgroup and the default values. Data in the other subgroups vary depending on the values specified in this subgroup.

A.5.3.2 Layer Thickness and Material Data Subgroup--

Table A-12 describes the layer thickness and material data necessary for the Landfill Module. The data consist of the layer thickness and the material number associated with each layer. The material numbers correspond to the order in which the material properties are read in as part of the Material Properties Subgroup described in Section A.5.3.4.

A.5.3.3 Liner Property Data Subgroup--

Liners are low permeability sheets of rubber or plastic materials which are used as barriers to vertical flow. A description of the liner property data can be found in Table A-13. There should be one set of data for each liner (LFCP(4)) in Table A-11. These data include the liner thickness, liner hydraulic conductivity, percent failure of the liner and the layer number containing the liner. The variables in this subgroup are presented in Table A-14.

A.5.3.4 Landfill Material Property Data Subgroup--

The landfill can consist of a number of different materials (the number specified by the value of LFCP(2) in Table A-11) with different hydrogeological properties. The properties for each of the materials are included in this subgroup. Details of the contents and formats of this subgroup are shown in Tables A-15 and A-16. When the landfill consists of more than one material, information about each material is input using an Array Subgroup. These materials are subsequently identified by the order in which the Array Subgroups appear. Thus, material number 4 would refer to the material that has properties included in the fourth Array Subgroup. The termination of data for each material is indicated by an END CARD. The end of the Landfill Material Property Data Subgroup is also indicated by an END CARD.

A.5.3.5 Hydrologic Data Subgroup--

A water balance approach is used to estimate the average infiltration rate over the duration of an "event." An event is defined as the typical period between the start of two sequential storms, and includes both the storm duration and the inter-storm interval. Table A-17 describes the contents and format of the Hydrologic Data Subgroup required to perform this balance. The hydrologic parameters are presented in Table A-18.

A.5.4 Chemical Data Group

The contents and format of the Chemical Data Group are shown in Table A-19. The first card is the GROUP SPECIFICATION CARD, with the code CHE in the first three columns. The second card is the SUBGROUP SPECIFICATION CARD, with the code ARR in the first three columns. This subgroup contains the array of information

Table A-11. CONTENTS AND FORMAT OF THE LANDFILL MODULE CONTROL DATA GROUP

Card	Contents	Format
V1	"LFL"	A3
CO2	"CON"	A3
CO3	CURVE, LFCP(I), I = 1,6	F10.0, 6I10
CO4	"END"	A3

Definition of Contents

"LFL"		Group Specification Card indicating the start of the Landfill Module Data Group.
CON		Subgroup Specification Card indication the start of the Landfill Module Control Data Subgroup.
CURVE		SCS curve number for moisture condition AMC-II.
LFCP(1)		Number of layers in the Landfill Module.
LFCP(2)		Number of different porous materials. Maximum permissible is 20.
LFCP(3)		Parameter indicating the type of relationship used for relative permeability versus saturation.
	1	van Genuchten functional parameters
	2	Brooks and Corey functional parameter
LFCP(4)		Number of liners in the landfill.
LFCP(5)		Number of seasons.
LFCP(6)		Parameter indicating method for calculating evapotranspiration. (Only one option is available in the current version of the code.)
	0	Seasonal potential evapotranspiration read in
LFCP(7)		Number of the layer which is the lateral drainage layer. Enter 0 if there is no lateral drainage layer.
"END"		End Card indicating the end of the Landfill Module Control Data Subgroup.

Table A-12. CONTENTS AND FORMAT OF THE LANDFILL MODULE LAYER THICKNESS AND MATERIAL DATA SUBGROUP

Card	Contents	Format
LA1	"LAY"	A3
LA2	LFLAYR(I), LPROP(I)	G10.0, I10
LA3	"END"	A3

Note: Card/line LA2 is repeated for each layer in the Landfill Module (LFCP(1) in Table A-11).

Definition of Contents

"LAY"	Subgroup Specification Card indicating the start of the Landfill Layer Thickness and Material Subgroup.
LFLAYR(I)	Thickness of layer I.
LPROP(I)	Material number for layer I corresponding to data read as part of the Material Properties Subgroup (see Section A.5.3.4).
"END"	End Card indicating the end of this subgroup.

about the values and/or the distributions and upper and lower bounds of up to 16 chemical-specific variables. The variables being input are identified by the value of the index I. The variables associated with each index I are shown in Table A-20. For example, a data card with I = 6 indicates that the card contains information about the base catalyzed hydrolysis rate constant for the chemical being simulated.

If any of the variables are specified to have an empirical distribution (NDSTPRM(I) = 6), then it is necessary to include the empirical distribution subgroup, discussed in Section A.4.5. If none of the chemical-specific variables have an empirical distribution, then this subgroup is not necessary.

A.5.5 Unsaturated Zone Flow Data Group

This group contains data required by the Unsaturated Zone Flow Module and consists of five subgroups. The Control Data Subgroup should be the first subgroup in the Unsaturated Zone Flow Data Group. The subgroups and the associated codes are listed below:

Table A-13. CONTENTS AND FORMAT OF THE LANDFILL MODULE LINER PROPERTY SUBGROUP

Card	Contents	Format
L1	"LIN"	A3
LA1	"LAY"	A3
LA2	LINER(I)	I5
LA3	"END"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
LI2	"END" (Material)	A3
LI3	"END"	A3

Note: Cards/lines A1-A3 and E1-E5 need to be repeated for each liner (i.e., LFCP(4) number of times). The Empirical Distribution Subgroup is needed only if one or more variables in the Array Subgroup has an empirical distribution.

Definition of Contents

"LIN"	Subgroup Specification Card indicating the start of the Landfill Liner Properties Data Subgroup.
"LAY"	Subgroup Specification Card indicating data containing layer number associated with liner properties.
LINER(I)	Layer number associated with the following data.
Array Subgroup	Subgroup defining the landfill liner properties variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of data for a liner (one such end card is required for each liner).
"END"	End Card indicating the end of this subgroup.

TABLE A-14. VARIABLES IN THE LANDFILL LINER PROPERTY ARRAY SUBGROUP

```
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

ARRAY VALUES
***         LANDFILL LINER VARIABLES

***            VARIABLE NAME                UNITS                DISTRIBUTION   PARAMETERS            LIMITS
***                                                                              MEAN      STD DEV    MIN      MAX
*****************************************************************************************************************************
 1 Thickness of liner (mills)                                          0      -999.     -999.     0.100E-08 -999.
 2 Hydraulic conductivity (cm/hr)                                      0      -999.     -999.     0.100      10.0
 3 Failure rate of liner (%)                                           0      -999.     -999.     0.000E+00  100.
END ARRAY

END LINER  1
END LINER DATA
```

Table A-15. CONTENTS AND FORMAT OF THE LANDFILL MODULE MATERIAL PROPERTY SUBGROUP

Card	Contents	Format
SA1	"SAT"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
SA2	"END" (Material)	A3
SA3	"END"	A3

Note: Cards/lines A1-A3 and E1-E5 need to be repeated for each material (i.e., LFCP(2) number of times). The Empirical Distribution Subgroup is needed only if one or more variables in the Array Subgroup has an empirical distribution.

Definition of Contents

"SAT"	Subgroup Specification Card indicating the start of the Landfill Material Data Subgroup.
Array Subgroup	Subgroup defining the landfill material variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of data for a material (one such end card is required for each material).
"END"	End Card indicating the end of this subgroup.

TABLE A-16. VARIABLES IN THE LANDFILL MATERIAL PROPERTY ARRAY SUBGROUP

```
SATURATED MATERIAL PROPERTY PARAMETERS FOR LANDFILL
ARRAY VALUES
***      LANDFILL MATERIAL VARIABLES
```

***	VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
***				MEAN	STD DEV	MIN	MAX
1	Sat hydraulic conduct	(cm/hr)	0	-999.	-999.	0.100E-10	0.100E+05
2	Porosity		0	-999.	-999.	0.100E-08	1.00
3	Residual water content		0	-999.	-999.	0.100E-08	1.00
4	Brooks and Corey exponent		0	-999.	-999.	0.000E+00	10.0
5	ALFA coeff for landfill	(1/cm)	0	-999.	-999.	0.000E+00	1.00
6	BETA - Van Genuchten exponent		0	-999.	-999.	0.000E+00	10.0

```
END ARRAY

END MATERIAL  1
END SATURATED MATERIAL PROPERTY DATA
```

Table A-17. CONTENTS AND FORMAT OF THE LANDFILL MODULE HYDROLOGY SUBGROUP

Card	Contents	Format
HY	"HYD"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
HY2	"END" (Season)	A3
HY3	"END"	A3

Note: Cards/lines A1-A3 and E1-E5 need to be repeated for each season (i.e., LFCP(5) number of times). The Empirical Distribution Subgroup is needed only if one or more variables in the Array Subgroup has an empirical distribution.

Definition of Contents

"HYD"	Subgroup Specification Card indicating the start of the Landfill Hydrology Data Subgroup.
Array Subgroup	Subgroup defining the landfill hydrology variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of data for a season (one such end card is required for each season).
"END"	End Card indicating the end of this subgroup.

TABLE A-18. VARIABLES IN THE LANDFILL HYDROLOGY ARRAY SUBGROUP
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

HYDROLOGY PARAMETERS
ARRAY VALUES
*** HYDROLOGY VARIABLES

*** VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
1 Precipitation (cm)		0	-999.	-999.	0.000E+00	-999.
2 Duration of event (days)		0	-999.	-999.	0.000E+00	-999.
3 Pan evaporation (cm)		0	-999.	-999.	0.000E+00	-999.

END ARRAY

END SEASON 1
END HYDROLOGY DATA

Table A-19. CONTENTS AND FORMAT OF THE CHEMICAL-SPECIFIC DATA GROUP

Card	Contents	Format
C1	"CHE"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
C2	"END"	A3

Definition of Contents

"CHE"	Group Specification Card indicating the start of the Chemical Data Group.
Array Subgroup	Subgroup defining the chemical variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of the Chemical Data Group.

Subgroup	Specification Code	Refer to Table
Control Data	CON	A-21
Layer Thickness and Material Data	MAT	A-22
Unsaturated Material Property Data	SAT	A-23
Soil Moisture Data	SOI	A-25

The first card of this group is the GROUP SPECIFICATION CARD and includes the code VFL in the first three columns. The next card is the first subgroup specification card. Data for each of these subgroups are described below. The end of this group is indicated by an END CARD.

A.5.5.1 Unsaturated Zone Flow Control Data Subgroup--

Table A-21 describes the Unsaturated Zone Flow Control Data Subgroup parameters. Data in the other subgroups vary depending on the options specified in the Control Data Subgroup. The termination of this subgroup is indicated by the END CARD.

TABLE A-20. VARIABLES IN THE CHEMICAL ARRAY SUBGROUP

CHEMICAL SPECIFIC VARIABLE DATA
ARRAY VALUES
*** CHEMICAL SPECIFIC VARIABLES

***	VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	PARAMETERS STD DEV	LIMITS MIN	LIMITS MAX
1	Solid phase decay coeff (1/yr)		-1	-999.	-999.	0.000E+00	0.100E+11
2	Diss phase decay coeff (1/yr)		-1	-999.	-999.	0.000E+00	0.100E+11
3	Overall chem dcy coeff (1/yr)		-1	-999.	-999.	0.000E+00	0.100E+11
4	Acid cataly hydrol rte(l/M-yr)		0	-999.	-999.	0.000E+00	-999.
5	Neutral hydrol rate cons(1/yr)		0	-999.	-999.	0.000E+00	-999.
6	Base cataly hydrol rte(l/M-yr)		0	-999.	-999.	0.000E+00	-999.
7	Reference temperature (C)		0	-999.	-999.	0.000E+00	100.
8	Normalized distrib coeff(ml/g)		0	-999.	-999.	0.000E+00	-999.
9	Distribution coefficient		-2	-999.	-999.	0.000E+00	0.100E+11
10	Biodegrad coef(sat zone)(1/yr)		0	-999.	-999.	0.000E+00	-999.
11	Air diffusion coeff (cm2/s)		0	-999.	-999.	0.000E+00	10.0
12	Ref temp for air diffusion (C)		0	-999.	-999.	0.000E+00	100.
13	Molecular weight (g/mole)		0	-999.	-999.	0.000E+00	-999.
14	Mole fraction of solute		0	-999.	-999.	0.100E-08	1.00
15	Solute vapor pressure (mm Hg)		0	-999.	-999.	0.000E+00	100.
16	Henry`s law cons (atm-m^3/M)		0	-999.	-999.	0.100E-09	1.00
17	Not in use		0	-999.	-999.	0.000E+00	1.00
18	Not in use		0	-999.	-999.	0.000E+00	1.00
19	Not in use		0	-999.	-999.	0.000E+00	1.00

END ARRAY

END CHEMICAL SPECIFIC VARIABLE DATA

Table A-21. CONTENTS AND FORMAT OF THE UNSATURATED ZONE FLOW MODULE CONTROL DATA GROUP

Card	Contents	Format
V1	"VFL"	A3
CO2	"CON"	A3
CO3	VFCP(I), I = 1,	5I10
CO4	"END"	A3

Definition of Contents

"VFL" Group Specification Card indicating the start of the Unsaturated Zone Flow Module Data Group.

CON Subgroup Specification Card indicating the start of the Unsaturated Zone Flow Module Control Data Subgroup.

VFCP(1) Number of nodes in the Unsaturated Zone Flow Module. The value of this parameter is currently generated in the code. Thus, the value in the input file is ignored.

VFCP(2) Number of different porous materials up to a maximum of 20. If the depth of the unsaturated zone is randomly generated in Monte Carlo mode, VFCP(2) must equal 1.

VFCP(3) Parameter indicating the type of relationship of relative permeability versus saturation.

1 van Genuchten functional parameters
2 Brooks and Corey functional parameter

VFCP(4) Parameter indicating the method of generating vertical discretization when the depth of the unsaturated zone is constant. This parameter is ignored in the current version of the code.

VFCP(5) Number of layers in the unsaturated flow system (up to a maximum of 20). If the depth of the unsaturated zone is randomly generated in Monte Carlo mode, VFCP(5) must equal 1.)

"END" End Card indicating the end of this subgroup.

Note that in Monte Carlo mode, the total depth of the unsaturated zone can be randomly generated by setting VFCP(2) and VFCP(5) to a value of one. VTCP(1) in Table A-27 must also be set to a value of one. In other words, only one homogeneous layer can have a Monte Carlo distribution associated with it.

A.5.5.2 Unsaturated Flow Module Layer Thickness and Material Data Subgroup--

Table A-22 describes the layer thickness and material data necessary for the Unsaturated Zone Flow Module. The data consist of the layer thickness and the material number associated with each layer. When only one layer is simulated, the layer thickness is equal to the total depth of the unsaturated zone and this parameter can have a Monte Carlo distribution assigned to it. The material numbers correspond to the material properties which are read in using the Material Properties Subgroup described in Section A.5.5.3.

A.5.5.3 Unsaturated Zone Flow Material Property Subgroup--

The unsaturated zone can consist of a number of different materials (the number specified by the value of VFCP(2) in Table A-21) with different hydrogeological properties. The properties for each of the materials are input using the Array and Empirical Subgroups in the Unsaturated Zone Material Property Subgroup, which is identified by the code SAT. Details of the contents and format of this subgroup are shown in Table A-23. The variables included in this subgroup are shown in Table A-24. Note that none of these variables can be derived (i.e., none have a distribution type of -1).

When the unsaturated zone consists of more than one material, information about each material is input using an Array Subgroup. These materials are subsequently identified by the order in which the Array Subgroups appear. Thus, the fourth Array Subgroup (after the Subgroup Specification Card) contains information about the properties of material number 4. The termination of data for each material is indicated by an END CARD. The end of the unsaturated materials data is also indicated by an END CARD.

A.5.5.4 Unsaturated Zone Flow Moisture Data Subgroup--

In order to solve the unsaturated zone flow problem, both the relationship between the relative permeability and water content and the relationship between pressure head and water content need to be specified for each material (refer to Section 3 of Salhotra et al. (1990)). The information needed to describe these relationships is provided in the Unsaturated Zone Moisture Data Subgroup, identified by the code SOI. The contents and format of this subgroup are described in Table A-25.

The van Genuchten parameters, alpha and beta, are <u>required</u> by the code to calculate the pressure head versus water content curve. The same parameters can be used to describe the relationship between relative permeability and water content by setting VFCP(3) equal to one in Table A-21. However, the code contains the option of using the Brooks and Corey relationship instead (VFCP(3)

Table A-22. CONTENTS AND FORMAT OF THE UNSATURATED FLOW MODULE LAYER THICKNESS AND MATERIAL DATA SUBGROUP

Card	Contents	Format
M1	"MAT"	A3
M2	VFLAYR(I), IPROP(I)	G10.0, I10
M3	"END"	A3

Note: Card/line M2 is repeated for each layer in the Unsaturated Flow Module (VFCP(5) in Table A-21).

Definition of Contents

"MAT"	Subgroup Specification Card indicating the start of the Unsaturated Flow Module Layer Thickness and Material Subgroup.
VFLAYR(I)	Thickness of layer I.
IPROP(I)	Material number for layer I corresponding to data read as part of the Material Data Subgroup (see Section A.5.5.3).
"END"	End Card indicating the end of this subgroup.

Table A-23. CONTENTS AND FORMAT OF THE UNSATURATED ZONE FLOW MODULE MATERIAL PROPERTY SUBGROUP

Card	Contents	Format
SA1	"SAT"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
SA2	"END" (Material)	A3
SA3	"END"	A3

Note: Cards/lines A1-A3 and E1-E5 need to be repeated for each material.

Definition of Contents

"SAT"	Group Specification Card indicating the start of the Unsaturated Zone Flow Module Material Subgroup.
Array Subgroup	Subgroup defining the material property variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of data for a material (one such end card is required for each material).
"END"	End Card indicating the end of this subgroup.

equal to 2 in Table A-21). If the Brooks and Corey option is selected, the exponent, n, must be specified in addition to the van Genuchten parameters.

The subgroup specification card is followed by VFCP(2) number of the Array Subgroups, one subgroup for each material. Table A-26 presents the definitions of the variables included in the Array Subgroup. None of the variables in this group can be derived (i.e., none have a distribution type of -1).

Note that the data for each material are read in the same sequence as in Table A-23. After the data for each material has been input, an END card is inserted. Finally, the end of the subgroup is also indicated by an END CARD.

TABLE A-24. VARIABLES IN THE UNSATURATED FLOW MATERIAL PROPERTY ARRAY SUBGROUP
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

SATURATED MATERIAL PROPERTY PARAMETERS
ARRAY VALUES
*** SATURATED MATERIAL VARIABLES

***	VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	STD DEV	LIMITS MIN	MAX
1	Sat hydraulic conduct (cm/hr)		0	-999.	-999.	0.100E-10	0.100E+05
2	Unsaturated zone porosity		0	-999.	-999.	0.100E-08	0.990
3	Air entry pressure head (m)		0	-999.	-999.	0.000E+00	-999.
4	Depth of the unsat zone (m)		0	-999.	-999.	0.100E-08	-999.

END ARRAY

END MATERIAL 1
END

Table A-25. CONTENTS AND FORMAT OF THE UNSATURATED ZONE FLOW MODULE MOISTURE DATA SUBGROUP

Card	Contents	Format
SI1	"SOI"	A3
A1-A3	Array Subgroup	(See Table A-5)
SI2	"END" (material)	A3
SI3	"END"	A3

Note: Card/line A1-A3 need to be repeated for each material.

Definition of Contents

"SOI"	Group Specification Card indicating the start of the Unsaturated Zone Flow Module Moisture Data Subgroup.
Array Subgroup	Subgroup defining the moisture-related variables.
"END"	End Card indicating the end of data for a material (one such end card is required for each material).
"END"	End Card indicating the end of this subgroup.

A.5.6 Unsaturated Zone Transport Data Group

The data required for the Unsaturated Zone Transport Module are divided into two subgroups. Each subgroup is handled in the same manner as was described for the subgroups of the Unsaturated Zone Flow Data Group. The subgroups included in the Unsaturated Zone Transport Data Group are:

Subgroup	Specification Code	Refer to Table
Control Data	CON	A-27
Transport Properties	TRA	A-28

The first card of this group is the GROUP SPECIFICATION CARD and includes the code VTL in the first three columns. The next card is the first SUBGROUP SPECIFICATION CARD. The contents and format of each of these subgroups are described below. The termination of the Unsaturated Zone Data Group is indicated by an END CARD.

TABLE A-26. VARIABLES IN THE UNSATURATED FLOW MOISTURE DATA ARRAY SUBGROUP
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

SOIL MOISTURE PARAMETERS
*** FUNCTIONAL COEFFICIENTS
ARRAY VALUES
*** FUNCTIONAL COEFFICIE VARIABLES

***	VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	STD DEV	LIMITS MIN	MAX
1	Residual water content		0	-999.	-999.	0.100E-08	1.00
2	Brooks and Corey exponent, EN		0	-999.	-999.	0.000E+00	10.0
3	ALFA van Genuchten coefficient		0	-999.	-999.	0.000E+00	1.00
4	BETA Van Genuchten coefficient		0	-999.	-999.	1.00	5.00

END ARRAY

END MATERIAL 1
END
END UNSATURATED FLOW

A.5.6.1 Unsaturated Zone Transport Control Data Subgroup--

The contents and format of the Control Data Subgroup are shown in Table A-27. The Control Data Subgroup should be the first subgroup included in the Unsaturated Zone Transport Group. Note that VTCP(1), the number of layers, is set equal to 1 if the depth of the unsaturated zone is generated from a Monte Carlo distribution in the Unsaturated Zone Flow Module. The end of this subgroup data is indicated by an END CARD.

A.5.6.2 Unsaturated Zone Transport Properties Subgroup--

The contents and format of the Transport Properties subgroup are described in Table A-28. Following the SUBGROUP SPECIFICATION CARD is one or more Array Subgroup that contains the values of the unsaturated zone transport variables. An Array Subgroup is required for each material layer. If any of the variables are specified to have an empirical distribution, then it is necessary to include the Empirical Distribution Subgroup (for details see Section A.4.5). An END CARD is used to indicate the end of data for each layer.

The multiple layers option is available only when the depth of the unsaturated zone is constant (i.e., not a Monte Carlo variable) in the Unsaturated Zone Flow Module. In the event that there is more than one transport layer, the sum of the individual layer thicknesses must equal the sum of the layer thicknesses specified in the Unsaturated Zone Flow Module. However, note that the number of layers and the corresponding thicknesses can differ between the two modules.

The definitions of the specific variables that comprise this subgroup are shown in Table A-29. Of the five variables shown, only the longitudinal dispersivity of the soil can be derived. The method by which it is derived is discussed in Section 4.4.3.1 of Salhotra et al. (1990). An END CARD indicates the end of the Transport Data Subgroup.

A.5.7 Aquifer Data Group

The contents and format of the Aquifer Data Group are shown in Table A-30. The first card is the GROUP SPECIFICATION CARD, with the code AQU included in the first three columns. Following this is an Array Subgroup, which contains information about the values and/or distributions of up to 18 aquifer-specific variables. The variables included in this subgroup are shown in Table A-31. With the exception of the source thickness, the variables are used only in the Saturated Zone Transport Module. The source thickness is used to satisfy the mass balance between the Unsaturated Zone (or the Source when the unsaturated zone is not simulated) and the Saturated Zone Transport Modules.

Ten of the aquifer variables can be either derived or directly input. These variables are the particle diameter, porosity, bulk density, source thickness, hydraulic conductivity, seepage velocity, retardation coefficient, and the longitudinal, lateral, and vertical dispersivities. The available options and the algorithms for each of them are explained in Section 5.5.3 of Salhotra et al. (1990).

Table A-27. CONTENTS AND FORMAT OF THE UNSATURATED ZONE TRANSPORT MODULE CONTROL DATA SUBGROUP

Card	Contents	Format
V1	"VTL"	A3
TC1	"CON"	A3
TC2	VTCP(I), I = 1,10	10I10
TC3	WTFUN	F10.0
TC4	"END"	A3

Definition of Contents

"VTL" Group specification card indicating the start of the Unsaturated Zone Transport Group.

"CON" Control card indicating the start of the Unsaturated Transport Control Subgroup.

VTCP(1) Number of layers used to simulate transport in the unsaturated zone (up to a maximum of 20). Note that the number of layers specified in the Unsaturated Zone Transport Module can be different from the number of layers specified in the Unsaturated Flow Module. VTCP(1) must be set equal to one if the depth of the unsaturated zone in the Unsaturated Flow Module is to be randomly generated in Monte Carlo mode.

VTCP(2) Number of time values at which concentration in the unsaturated zone is to be evaluated. This variable, which corresponds to the number of control points in the convolution integral for coupling the unsaturated and saturated zones, is not used when the model is run in steady-state. In the current version of the preprocessor, this value is set to 20.

VTCP(3) Dummy integer. Not used in the current version of the model.

VTCP(4) Type of scheme used to evaluate transport in the unsaturated zone. Note that the Stehfest algorithm is recommended when the ratio of layer thickness to longitudinal dispersivity is less than 20.

1 Stehfest numerical inversion algorithm
2 Convolution integral approach

(continued)

Table A-27. CONTENTS AND FORMAT OF THE UNSATURATED ZONE TRANSPORT MODULE CONTROL DATA SUBGROUP (concluded)

	Definition of Contents
P(5)	For VTCP(4) = 1, the number of terms governing the accuracy of the Stehfest algorithm. It must be a positive even integer. A value of 18 is suggested as an initial trial value. For VTCP(4) = 2, the number of increments used in the temporal discretization of convolution integral approach (a value of 10 is recommended).
VTCP(6)	Number of points in the Lagrangian scheme used for interpolating concentration values (a value of 3 is recommended).
VTCP(7)	Number of Gauss points used in Gauss-Legendre numerical integration of the convolution values (a value of 104 is recommended).
VTCP(8)	Number of segments for the numerical approximation of the convolution integral (a value of 2 is recommended).
VTCP(9)	Type of source boundary condition. In the current version of the code, the value of this parameter is automatically set in subroutine DEFAULTS.FOR, based on the values of other input parameters.
VTCP(10)	Parameter indicating if time values for computing concentration in the unsaturated zone are to be generated. This variable is not used when the model is run in steady-state. It is automatically set to 1 (i.e., yes), the recommended value, in the current version of the preprocessor.
WTFUN	Value of weighting factor used to generate time step values for evaluating concentration in the unsaturated zone. This variable, which is not used when the model is run in steady-state, is automatically set to 1.2 in the current version of the preprocessor.
"END"	End Card indicating the end of this data subgroup.

Table A-28. CONTENTS AND FORMAT OF THE UNSATURATED ZONE TRANSPORT MODULE PROPERTIES SUBGROUP

Card	Contents	Format
T1	"TRA"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
T2	"END" (Layer)	A3
SA3	"END"	A3

Note: Cards/lines A1-A3 and E1-E5 need to be repeated for each layer.

Definition of Contents

"TRA"	Group Specification Card indicating the start of the Unsaturated Zone Transport Module Data Subgroup.
Array Subgroup	Subgroup defining the transport variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of data for a layer (one such end card is required for each layer).
"END"	End Card indicating the end of this subgroup.

If any of the variables in this group are assigned an empirical distribution (NDSTPRM(I) = 6), then it is necessary to include the Empirical Distribution Subgroup (see Section A.4.5). END CARDS are required to indicate the termination of both the Array and the Empirical Subgroups. A final END CARD indicates the end of the Aquifer Data Group.

A.5.8 Surface Water Data Group

The contents and format of the Surface Water Data Group are shown in Table A-32. The first card is the GROUP SPECIFICATION CARD with the code SUR in the first three columns. This is followed an Array Subgroup that contains information about the values/distributions of 13 variables, two of which are not used in the current version of the model (see Table A-33). If any of these

TABLE A-29. VARIABLES IN THE UNSATURATED TRANSPORT PROPERTIES ARRAY SUBGROUP
444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

TRANSPORT PARAMETER
ARRAY VALUES
*** UNSATURATED TRANSPOR VARIABLES

***	VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	STD DEV	LIMITS MIN	MAX
1	Thickness of layer (m)		0	-999.	-999.	0.100E-08	-999.
2	Longit disper of layer (m)		-1	-999.	-999.	0.000E+00	0.100E+05
3	Percent organic matter		0	-999.	-999.	0.000E+00	100.
4	Bulk dens of soil layer (g/cc)		0	-999.	-999.	0.100E-01	5.00
5	Biological decay coeff (1/yr)		0	-999.	-999.	0.000E+00	-999.

END ARRAY

END LAYER 1
END UNSATURATED TRANSPORT PARAMETERS
END TRANSPORT MODEL

Table A-30. CONTENTS AND FORMAT OF THE AQUIFER-SPECIFIC DATA GROUP

Card	Contents	Format
Q1	"AQU"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
Q2	"END"	A3

Definition of Contents

"AQU"	Group Specification Card indicating the start of the Aquifer Data Group.
Array Subgroup	Subgroup defining the aquifer variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of this data group.

variables are specified to have an empirical distribution, then it is necessary to include the Empirical Distribution Subgroup. When running the Surface Water Module, the user must chose an exposure route. Figure A.4 shows the three options available. The choice is specified in the General Data Group. The end of the group is indicated by an END CARD.

A.5.9 Air Emissions and Dispersion Data Group

The Air Emissions and Dispersion Data Group may consist of up to three subgroups. The Array and Empirical Subgroups are used to specify values and distributions for air emissions and dispersion model variables. The third subgroup, the Air Dispersion Module Control Subgroup discussed in Section A.5.9.1, defines control options when the air dispersion model is used.

The first card of this group is the GROUP SPECIFICATION CARD and includes the code AIR in the first three columns. The next set of cards, shown in Table A-34, includes an Array Subgroup that contains information about the values/distributions of up to 18 variables (shown in Table A-35). Note that if any of these variables are specified to have an empirical distribution, then it is necessary to include the empirical subgroup.

TABLE A-31. VARIABLES IN THE AQUIFER DATA ARRAY SUBGROUP
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444

AQUIFER SPECIFIC VARIABLE DATA
ARRAY VALUES
*** AQUIFER SPECIFIC VARIABLES

*** VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS MEAN	STD DEV	LIMITS MIN	MAX
1 Particle diameter (cm)		0	-999.	-999.	0.100E-08	100.
2 Aquifer porosity		-2	-999.	-999.	0.100E-08	0.990
3 Bulk density (g/cc)		-1	-999.	-999.	0.100E-01	5.00
4 Aquifer thickness (m)		0	-999.	-999.	0.100E-08	0.100E+06
5 Mixing zone depth (m)		-1	-999.	-999.	0.100E-08	0.100E+06
6 Hydraulic conductivity (m/yr)		-2	-999.	-999.	0.100E-06	0.100E+09
7 Hydraulic Gradient		0	-999.	-999.	0.100E-07	-999.
8 Grndwater seep velocity (m/yr)		-2	-999.	-999.	0.100E-09	0.100E+09
9 Retardation coefficient		-1	-999.	-999.	1.00	0.100E+09
10 Longitudinal dispersivity (m)		0	-999.	-999.	0.100E-02	0.100E+05
11 Transverse dispersivity (m)		0	-999.	-999.	0.100E-02	0.100E+05
12 Vertical dispersivity (m)		0	-999.	-999.	0.100E-02	0.100E+05
13 Temperature of aquifer (C)		0	-999.	-999.	0.000E+00	100.
14 pH		0	-999.	-999.	0.300	14.0
15 Organic carbon content (fract)		0	-999.	-999.	0.100E-05	1.00
16 Receptor distance from site(m)		0	-999.	-999.	1.00	-999.
17 Angle off center (degree)		0	-999.	-999.	0.000E+00	360.
18 Well vertical distance (m)		0	-999.	-999.	0.000E+00	-999.

END ARRAY

END AQUIFER SPECIFIC VARIABLE DATA

Table A-32. CONTENTS AND FORMAT OF THE SURFACE WATER DATA GROUP

Card	Contents	Format
SU1	"SUR"	A3
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
SU2	"END"	A3

Definition of Contents

"SUR"	Group Specification Card indicating the start of the Surface Water Data Group.
Array Subgroup	Subgroup defining the surface water variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of this data group.

A.5.9.1 Air Dispersion Module Control Data Subgroup--

The Control Data Subgroup is identified by a SUBGROUP SPECIFICATION CARD with the code CON in the first three columns. The contents and format of the subgroup are shown in Table A-36. The subgroup is required only if the air dispersion module is used. Note that the values for wind speed and the value for FMAT are only read when IFREQ equals 1. The available options are shown in Figure A.5.

If the frequency-weighting approach is used to calculate long-term dispersion (IFREQ = 1), frequency data are read from the file FREQ.IN. The file contains joint frequencies for all combinations of wind speed, direction, and stability. For the usual configuration of 16 wind direction sectors, 6 wind speeds, and 6 stability classes 576 (i.e., 16 x 6 x 6) joint frequency entries are required. Typically this joint frequency distribution is available as STAR (Stability Array Data) summaries for airports. The general structure of the data is illustrated in Table A-37. Since users may have this matrix of data in different formats, MULTIMED allows some flexibility in the format. The formats for each line of data are specified by the variable FMAT on Card AR5 (Table A-36). The end of this subgroup is indicated by the END CARD. The completion of the Air Emissions and Dispersion Data Group is indicated by the END CARD.

TABLE A-33. VARIABLES IN THE SURFACE WATER DATA ARRAY SUBGROUP
4444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444444
SURFACE WATER MODULE VARIABLE DATA
ARRAY VALUES
*** SURFACE WATER MODULE VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
		MEAN	STD DEV	MIN	MAX	
1 Channel slope	(m/m)	0	-999.	-999.	0.100E-08	-999.
2 Stream depth	(m)	0	-999.	-999.	0.300E-01	-999.
3 unused at present		0	-999.	-999.	0.000E+00	0.000E+00
4 Mannings roughness coefficient		0	-999.	-999.	0.100E-08	1.00
5 Temperature of stream	(C)	0	-999.	-999.	0.000E+00	100.
6 Sediment concentration	(mg/l)	0	-999.	-999.	0.100E-08	-999.
7 Stream pH		0	-999.	-999.	0.300	14.0
8 Fract organic carbon in sedmt		0	-999.	-999.	0.100E-08	1.00
9 Wind speed at elev z	(m/s)	0	-999.	-999.	0.000E+00	200.
10 Elev of wind speed measure	(m)	0	-999.	-999.	0.100E-08	-999.
11 Fract of fish which is lipid		0	-999.	-999.	0.100E-08	1.00
12 unused at present		0	-999.	-999.	0.000E+00	0.000E+00
13 Stream flow	(m^3/s)	0	-999.	-999.	0.100E-08	-999.

END ARRAY

END SURFACE WATER MODULE VARIABLE DATA

Table A-34. CONTENTS AND FORMAT OF THE AIR EMISSION AND DISPERSION DATA GROUP

Card	Contents	Format
AIR	"AIR"	A3
AR2-AR6	Air Dispersion Control Subgroup	(See Table A-36)
A1-A3	Array Subgroup	(See Table A-5)
E1-E5	Empirical Distribution Subgroup	(See Table A-6)
AR7	"END"	A3

Definition of Contents

"AIR"	Group Specification Card indicating the start of the Air Emission and Dispersion Data Group.
Array Subgroup	Subgroup defining the air variables.
Empirical Distribution Subgroup	Subgroup defining any empirical distributions.
"END"	End Card indicating the end of this data group.

TABLE A-35. VARIABLES IN THE AIR EMISSION AND DISPERSION DATA ARRAY 4444444444444444444444444444444444444444444444444444444444444444444444

AIR MODULE VARIABLE DATA

ARRAY VALUES

*** AIR MODULE VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION		PARAMETERS	LIMITS
		MEAN	STD DEV	MIN	MAX
1 Depth of soil cover	(cm)	0	-999.	-999.	0.000E+00 0.000E+00
2 Temper of waste disp unit	(C)	0	-999.	-999.	0.000E+00 0.000E+00
3 Porosity of unit		0	-999.	-999.	0.000E+00 0.000E+00
4 Water content		0	-999.	-999.	0.000E+00 0.000E+00
5 Gamma factor		0	-999.	-999.	0.000E+00 0.000E+00
6 Mu exponent		0	-999.	-999.	0.000E+00 0.000E+00
7 Sigma exponent		0	-999.	-999.	0.000E+00 0.000E+00
8 Atmos pump correction factor		0	-999.	-999.	0.000E+00 0.000E+00
9 Empirical enhancement factor		0	-999.	-999.	0.000E+00 0.000E+00
10 5 m/s height of rise	(m)	0	-999.	-999.	0.000E+00 0.000E+00
11 Decay coeff in air	(s^-1)	0	-999.	-999.	0.000E+00 0.000E+00
12 Receptor dist frm landfill	(m)	0	-999.	-999.	0.000E+00 0.000E+00
13 Receptor angl frm source	(rad)	0	-999.	-999.	0.000E+00 0.000E+00
14 Elevation of receptor	(m)	0	-999.	-999.	0.000E+00 0.000E+00
15 Mixing height	(m)	0	-999.	-999.	0.000E+00 0.000E+00
16 Std dev of wind elev ang	(rad)	0	-999.	-999.	0.000E+00 0.000E+00
17 Constant wind speed	(m/s)	0	-999.	-999.	0.000E+00 0.000E+00
18 Constant stability condition		0	-999.	-999.	0.000E+00 0.000E+00

END ARRAY

END AIR MODULE VARIABLE DATA

Table A-36. CONTENTS AND FORMAT OF THE AIR DISPERSION CONTROL DATA SUBGROUP

Card	Contents	Format
AR2	"CON"	A3
AR3	ISTBL, ISIGZ, IFREQ	3I5
AR4	(U(I), I = 1,6)	6F10.0
AR5	FMAT	A80
AR6	"END"	A3

Definition of Contents

"CON" Control card indication start of the Air Dispersion Control Subgroup (required only if air dispersion is simulated).

ISTBL Flag indication if terrain correction is stability dependent.
- 0 Stability-independent terrain correction
- 1 Stability-dependent terrain correction

ISIGZ Flag for vertical dispersion coefficient method.
- 0 The Pasquill-Gifford method
- 1 The turbulence-intensity method

IFREQ Flag indicating mode for calculation of oncentrations.
- 0 Concentrations are calculated assuming a constant wind in the direction of the receptor
- 1 Wind-stability frequency-weighting approach used

U(I) Wind speeds for each wind speed class (required only if IFREQ = 1).

FMAT Format for the data in the file containing wind-stability frequency data (required only if IFREQ = 1). The general structure of this file is illustrated in Table A-37.

"END" End Card indicating the end of this data subgroup.

Table A-37. GENERAL STRUCTURE OF THE WIND-STABILITY FREQUENCY FILE (FREQ.IN)

Wind Direction Sector	
1	Frequencies for six wind speed classes, sector 1, stability class A.
2	Frequencies for six wind speed classes, sector 2, stability class A.
3	Frequencies for six wind speed classes, sector 3, stability class A.
4	Frequencies for six wind speed classes, sector 4, stability class A.
5	Frequencies for six wind speed classes, sector 5, stability class A.
6	Frequencies for six wind speed classes, sector 6, stability class A.
7	Frequencies for six wind speed classes, sector 7, stability class A.
8	Frequencies for six wind speed classes, sector 8, stability class A.
9	Frequencies for six wind speed classes, sector 9, stability class A.
10	Frequencies for six wind speed classes,sector 10, stability class A.
11	Frequencies for six wind speed classes,sector 11, stability class A.
12	Frequencies for six wind speed classes,sector 12, stability class A.

APPENDIX B

SUBROUTINES INCLUDED IN MULTIMED

Subroutine	Called By	Description
Input/Output Routines		
ADISRD	BATIN	Reads input data necessary to run the Air Emissions Module and the Air Dispersion Module.
AIRIN	MAIN	Interactive preprocessor for Air Dispersion Module.
BATIN	MAIN	The batch-run input processor that reads from a user-specified file the values of variables and parameters updated from their default values.
CHKEND	BATIN, READLF	Checks for the end of a data group.
COMRD	ADISRD, AIRIN	Searches for data lines in input file. Separates connects from data input data file.
FRQPLT	OUTFOR	Prints a CDF and/or PDF to output file.
FRQTAB	OUTFOR	Prints a table of statistics to the output file.
ICHECK	READZ, READ3 BATIN, READLF	Separates data for connections in input data file.
LEFTJT	PRTINP, BATIN	Left justifies character variables.
MODCHK	MAIN	Flags which modules are to be run for Monte Carlo simulations.
OPENF	MAW	Opens files. Checks to see if they exist.
OUTFOR	MAIN	Outputs single statistics, frequency distribution tables, CDF tables, and printer plots.
Subroutine	Called By	Description
PRINTO	MAIN, PRTOUT, PRNTVZ	Outputs the distribution type, mean, standard deviation, and maximum and minimum allowed values for all the variables which can be generated by Monte Carlo routines.
PRNEMP	PRTOUT, PRNTVZ	Prints empirical distributions to output file.
PRNTIN	PRTINP, PRTOUT	Writes out General Data Group to the output file.
PRNTVZ	PRTINP	Outputs model parameters for the

		Unsaturated Zone Flow and Transport Modules to the computer-generated batch input file.
PRTINP	MAIN	Outputs model parameters to the computer-generated batch input file.
PRTOUT	MAIN	Outputs Monte Carlo information to output file.
READ2	BATIN, ADISRD, READLF	Reads in array values as part of the batch input preprocessor.
READ3	BATIN, ADISRD, READLF	Reads in empirical distributions as part as the batch input preprocessor.
READLF	BATIN	Reads in Landfill Source Data.
SOPEN	MAIN	Open output files containing Monte Carlo output. These are the *.VAR and *.OUT files.
<u>Saturated Zone Module</u>		
DBK1	STEADY	Calculates the modified Bessel function.
CONVO2	GWCALC	Couples Unsaturated Zone and Saturated Zone Modules using the convolution approach.
CPCAL	CONVO2	Evaluates saturated zone concentrations at time `T minus tau' for the convolution integral approach.

ERFC	TRANSP	Computes the complementary error function.

Subroutine	Called By	Description
FUNCT1	GW2DFT, QROMB, TRAPZD	Evaluates the integrand in the analytical solution.
GWCALC	MAIN	Main calling routine for saturated zone model. Sudicky's analytical solution for three-dimensional mass transport problem with a gaussian-distributed source.
GW2DFS	GWCALC, GW3DPS	Analytic solution to the saturated steady-state, two-dimensional, transport model with a continuous gaussian source using the Gauss-Legendre quadrature integration scheme.
GW2DFT	GWCALC, CPCAL, GW3DPT	Analytic solution to the saturated, unsteady-state, two-dimensional, transport model with a continuous gaussian source using the Gauss-Legendre quadrature integration scheme.
GW3DPS	GWCALC	Evaluates saturated, steady-state, three-dimensional transport from a continuous gaussian source. Allows for the effects of partial penetration.
GW3DPT	GWCALC, CPCAL	Evaluates saturated, unsteady-state, three-dimensional transport from a continuous gaussian source. Allows for partial penetration effects.
PATCH	MAIN	Solves for transport in the saturated zone assuming a patch source.
QROMB	GW2DFT	Preforms integration using Romberg's method of order 2K (e.g., K = 2 is Simpson's rule).
STEADY	PATCH	Steady-state solution for contaminant transport in the saturated zone when using a patch source.

TMGEN1	INITVT	Evaluates times used in convolution integral to couple the unsaturated zone and saturated zone transport solutions (for constant source).
Subroutine	Called By	Description
TMGEN2	INITVT	Evaluates times used in the convolution integral to couple the unsaturated zone and saturated zone transport solutions (for pulse source).
TMGEN3	INITVT	Evaluates times used in the convolution integral to couple the unsaturated zone and saturated zone transport solutions (for decaying source).
TRANSP	PATCH	Transient solution for contaminant transport in the saturated zone while using a patch source.
TRAPZD	QROMB	Computes the nth stage of refinement of an extended trapezoidal rule.
Unsaturated Zone Transport Module		
ADISPR	VTCALC	Computes concentrations based on the steady-state, advective dispersive equation with first order decay.
COEF	VTCALC	Generates coefficients of transformed solution for each layer.
CONVO1	VTCALC	Evaluates layered unsaturated zone transport solution by the convolution method.
DERFC	EXPERF	Computes complementary error function with real arguments.
DGAUSS	SOLBT, GW2DFS, STEADY, TRANSP	Computes the first N roots and weight factors for the Gauss-Legendre quadrature integration scheme.
EVAL	SOLBT	Evaluates functional values at Gauss integration points.

EXPD	EXPERF	Computes the exponential function. Set function to zero for agreements less than -170.
EXPERF	SOLAY1	Evaluates the product of an exponential function and the complementary error function with real arguments.
FACTR	LINV	Function which calculates the factorial of a number.
Subroutine	Called By	Description
LAGRNG	SOLBT	Lagrangian interpolation scheme.
LAYAVE	INITVT	Evaluates average saturation and porosity for each layer in the Unsaturated Transport Module.
LINV	INITVT	Evaluates coefficients for Stehfest algorithm.
SOLAY1	VTCALC, SOLBT	Analytical unsaturated transport solution for the first layer.
SOLBT	VTCALC, CONVO1	Evaluates unsaturated zone concentrations at the bottom of each layer at specific time intervals.
STEHF	VTCALC	Evaluates the inverse of the Laplace transform for solute transport in layered media.
VTCALC	MAIN	The main calling routine for the analytical solution of transport through the unsaturated zone.
Unsaturated Zone Flow Module		
FPSI1	RAPSON	Evaluates pressure head based upon relationship between pressure head and hydraulic conductivity and water content.

RAPSON	VFCALC	Determines pressure head corresponding to specific flux using modified Newton-Raphson iteration.
VFCALC	MAIN	Main calling routine for the one-dimensional Unsaturated Zone Flow Module.
WCFUN	VFCALC	Evaluates the water content-pressure head relationship.

Air Emission and Dispersion Module

AIRDIS	MAIN	Computes the ground-level concentration at receptors located downwind of the landfill.
ARCALC	MAIN	Calculates the emission rates from the waste disposal unit to the atmosphere.

Subroutine	Called By	Description
SIGMAZ	AIRDIS	Computes vertical dispersion coefficient.
VIRT	AIRDIS	Computes effective source area and locates the virtual source.

Surface Water Module

CINTER	SWCALC	Computes the fraction of the steady-state continuous mass leaching out of the waste disposal unit that enters the stream.
CMIX	SWCALC	Calculates the instream dilution due to complete near-field mixing of the groundwater plume.
DRINK	SWCALC	Calculates the reduction in stream contaminant concentration due to sedimentation in a water treatment plant.
FISH	SWCALC	Calculates the bioaccumulation of toxics in fish.
REOX	INITST	Calculates the reaeration coefficient, using either the Owens, O'Conner-Dobbins or Churchill formula, depending on the stream depth and/or velocity.
SWCALC	MAIN	Main calling routine for Surface Water Module.

Landfill Source Module

DISC	INITVF	Discretizes the landfill layers and unsaturated zone layers into a one dimensional grid for computing pressure head.
EVPT	LFCALC	Computes actual evapotranspiration using a limiting soil moisture calculation.
LFCALC	MAIN	Main calling routine for the Landfill Module.
LINER1	INITLF	Computes the effective permeability of a landfill layer with a synthetic liner.

Subroutine	Called By	Description
PERC	LFCALC	Computes pressure head, water content, and saturation distribution below a lateral drain.
RUNOFF	LFCALC	Computes runoff by SCS curve number method modified to include the soil moisture.

Initialization Routines

TRANS	SWCALC	Calculates the contaminant concentration in the stream at the location of the drinking water treatment plant intake. Assumes first order decay.
INITAR	MAIN	Assigns the input values or values generated by the Monte Carlo routines to the variable names used in the air emissions and dispersion models. Also calculates coefficients needed by the models.
INITGW	MAIN	Assigns the input variables or values generated by Monte Carlo routines to the variable names used in the saturated zone model. Calculates aquifer, chemical, and source constants.
INITLF	INITVF	Assigns the input variables or values generated by Monte Carlo routines to the variable modes used in the Landfill Model.
INITST	MAIN	Assigns the input values or values generated by the Monte Carlo routines to the variable names used in the Surface Water Module. Also calculates coefficients needed by the module.
INITVF	MAIN	Assigns the input variables or values generated by the Monte Carlo routines to the variable names used in the Unsaturated Flow Module. The initial conditions and coordinate system for the Unsaturated Flow Module are defined here.

INITVT	MAIN	Assigns the Unsaturated Transport input variables or values generated by Monte Carlo routines to their variable names. Assigns retardation and saturation to the appropriate transport variables.

Subroutine	Called By	Description
Monte Carlo Routines		
ANRMRN LOGNOR	NORMAL	Generates a (0,1) normally distributed random number.
CALLS	UNCPRO	Calls the prescribed random number generator for each parameter which is used in the Monte Carlo simulation.
COUNT	MAIN	Count the number of parameters which are to be Monte Carloed.
EMPCAL	CALLS	Generates a random number from an empirical distribution. EMPCAL generates a uniform random number between 0-1 and uses it to interpolate for a value using the piecewise linear cumulative frequency distribution input by the user.
EXPRN	EXPRND	Generates an exponentially distributed random number with a mean of 1.
EXPRND	CALLS	Generates an exponentially distributed random number with a specified mean.

LOGNOR	CALLS	Generates a lognormally distributed random number with a specified mean and standard deviation. The input mean and standard deviation are in arithmetic space.
LOG10U	CALLS	Generates uniformly distributed log10 numbers between 0-1, then transforms them to a range specified by the user.
NORMAL	CALLS	Generates a (x,σ)normally distributed random number where x is the mean and σ is the standard deviation.
PRMLIS	CHMOD, AQMOD, SOMOD, VTMOD, VFMOD, ARMOD, STMOD	In the interactive mode, lists the present, minimum, and maximum values and distribution values for the user-specified variables.
RANSET	MAIN	Initializes the random number generator.
TRANSB	CALLS	Transforms a number from SB space to normal space or from normal space to SB space.
Subroutine	Called By	Description
TRNLOG	CALLS	Transforms the mean and standard deviation in the arithmetic space (original data) to mean and standard deviation in logarithmic (normal) space.
UNCPRO	MAIN	Generates random values for the model parameters. It also writes to the output file if any errors occur when generating the random values.
UNFRN	ANRMRN, LOG10U UNIFRM, EXPRN	Generates a (0,1) uniformly distributed random number.
UNIFRM	CALLS, EMPCAL	Generates a uniformly distributed random number between a user-specified minimum and maximum.

Subroutines to Set Default Values and Interactive Routines

AQNAMS	MAIN	Sets Aquifer Data Group variable and label names.
ARNAMS	MAIN	Sets Air Data Group variable and label names.
CHNAMS	MAIN	Sets Chemical Data Group variable and label names.
DEFAULTS	MAIN	Sets special default values to lock out certain functions.
LFNAMS	MAIN	Sets Landfill Data Group variable and label names.
SONAMS	MAIN	Sets Source Data Group variable and label names.
STNAMS	MAIN	Sets Surface Water Data Group variable and label names.

VFNAMS	MAIN	Sets Unsaturated Flow Data Group variable and label names.
VTNAMS	MAIN	Sets Unsaturated Transport Data Group variable and label names.
ZIPI	BATIN	Used when reading batch files.

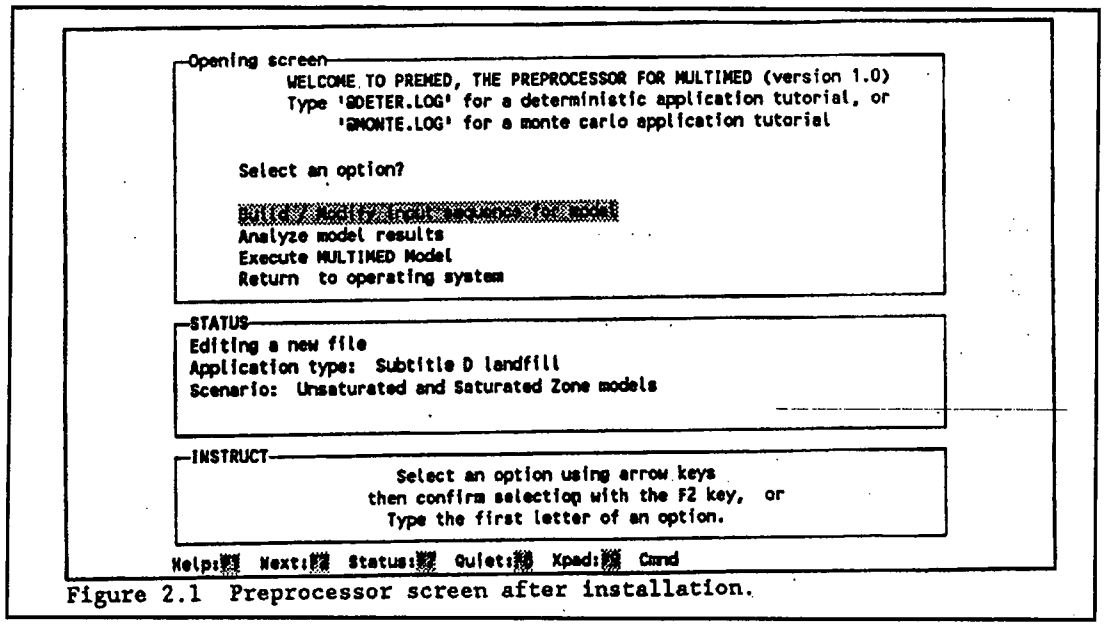


Figure 2.1 Preprocessor screen after installation.

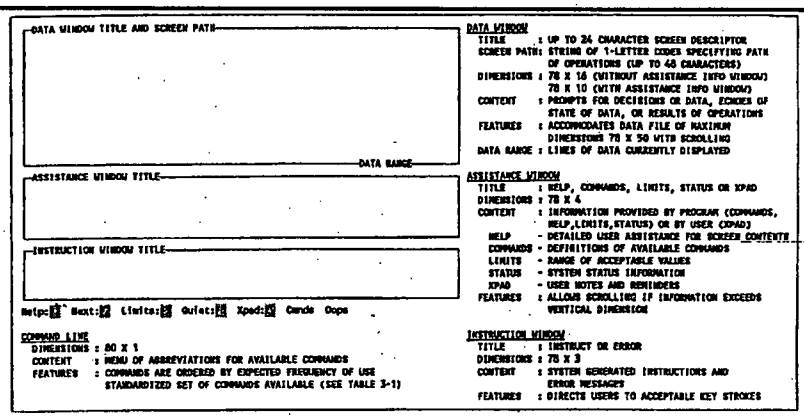


Figure 3.1 Screen format utilized by the pre- and postprocessor.

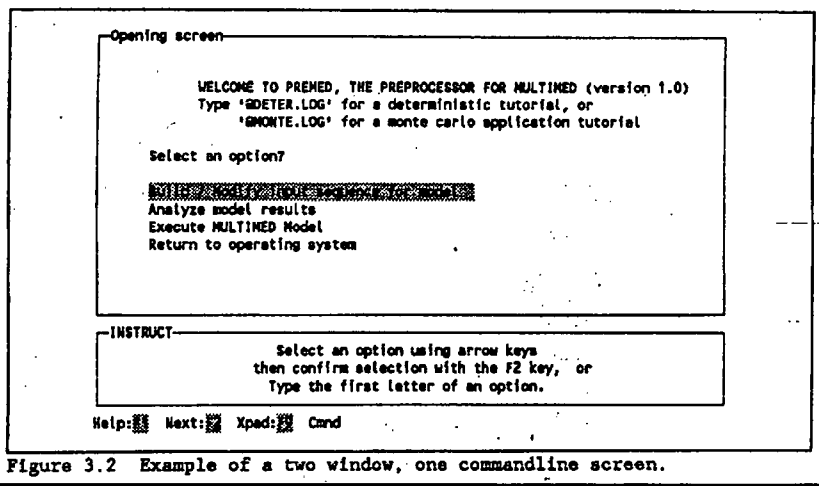


Figure 3.2 Example of a two window, one commandline screen.

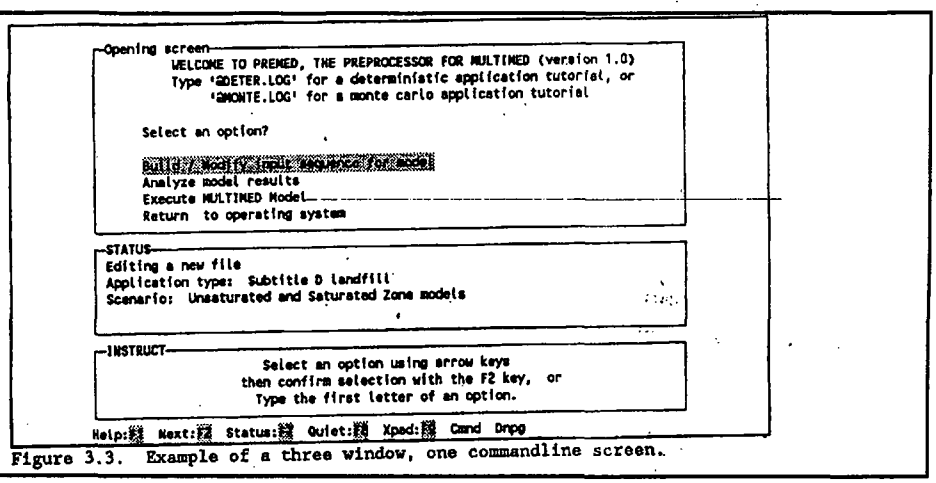


Figure 3.3. Example of a three window, one commandline screen.

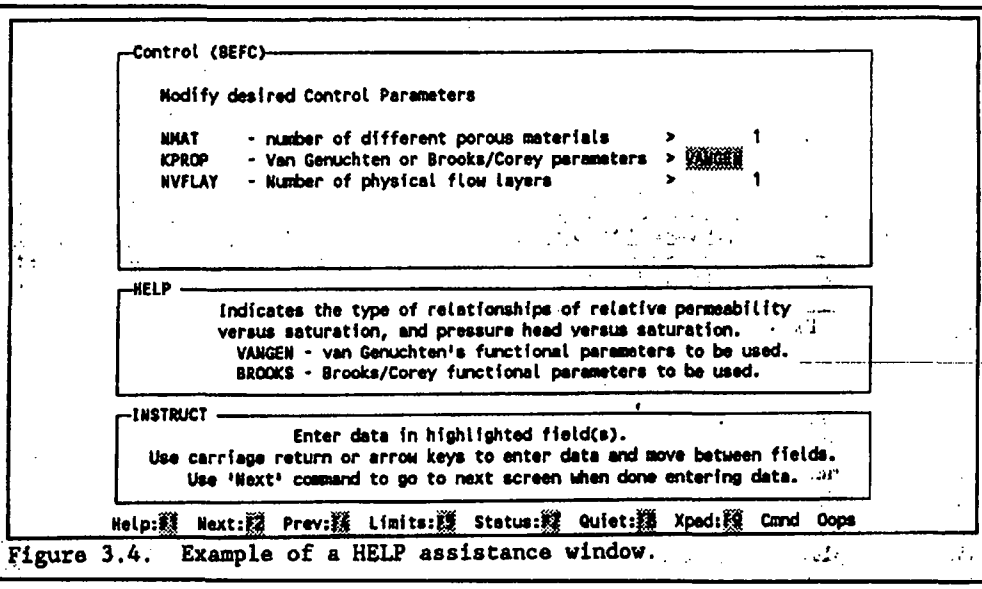


Figure 3.4. Example of a HELP assistance window.

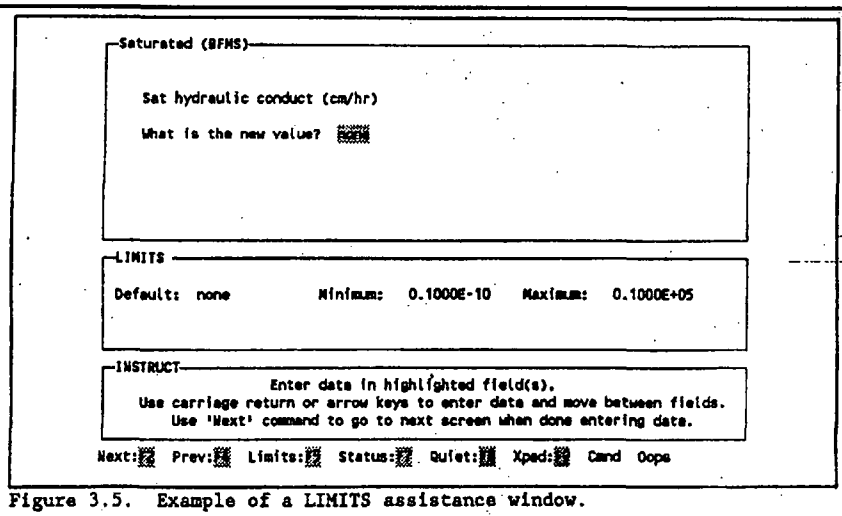


Figure 3.5. Example of a LIMITS assistance window.

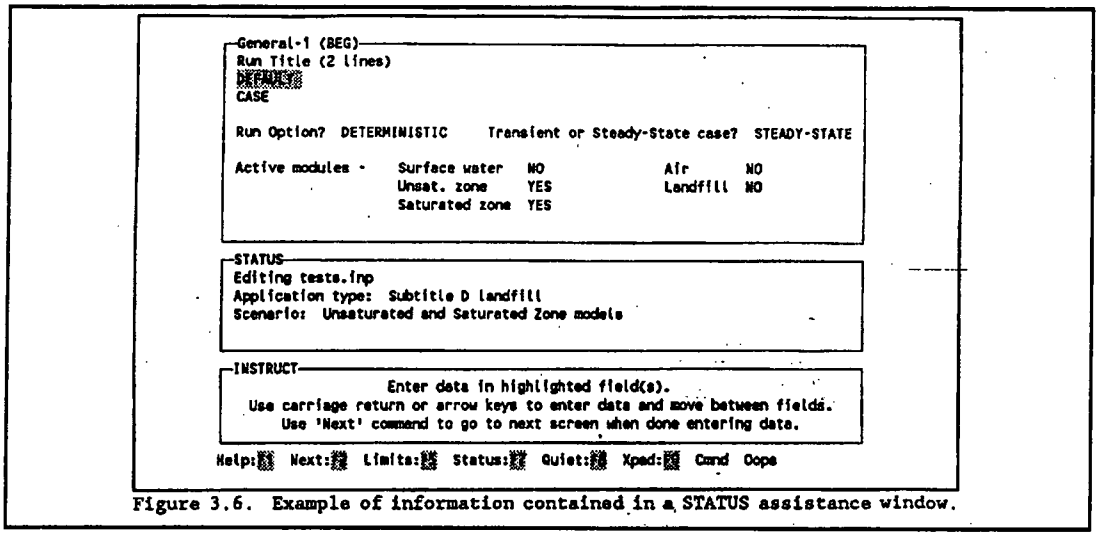


Figure 3.6. Example of information contained in a STATUS assistance window.

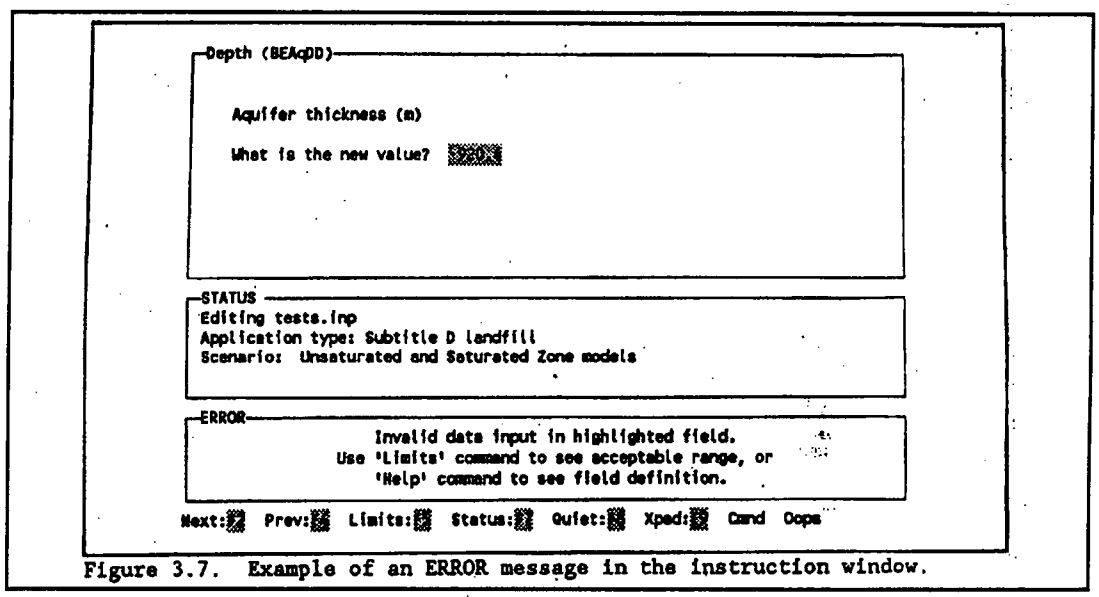


Figure 3.7. Example of an ERROR message in the instruction window.

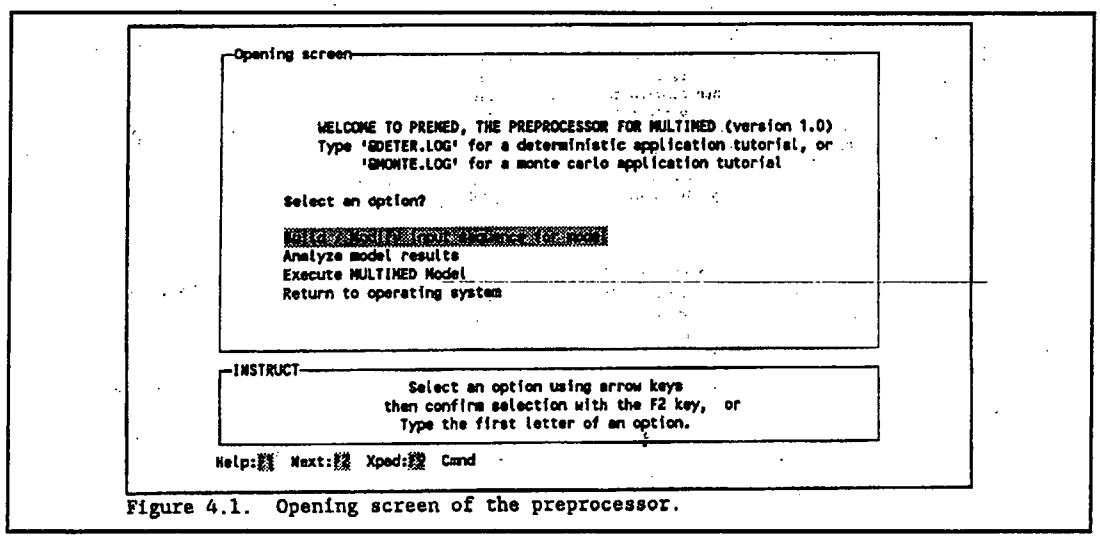


Figure 4.1. Opening screen of the preprocessor.

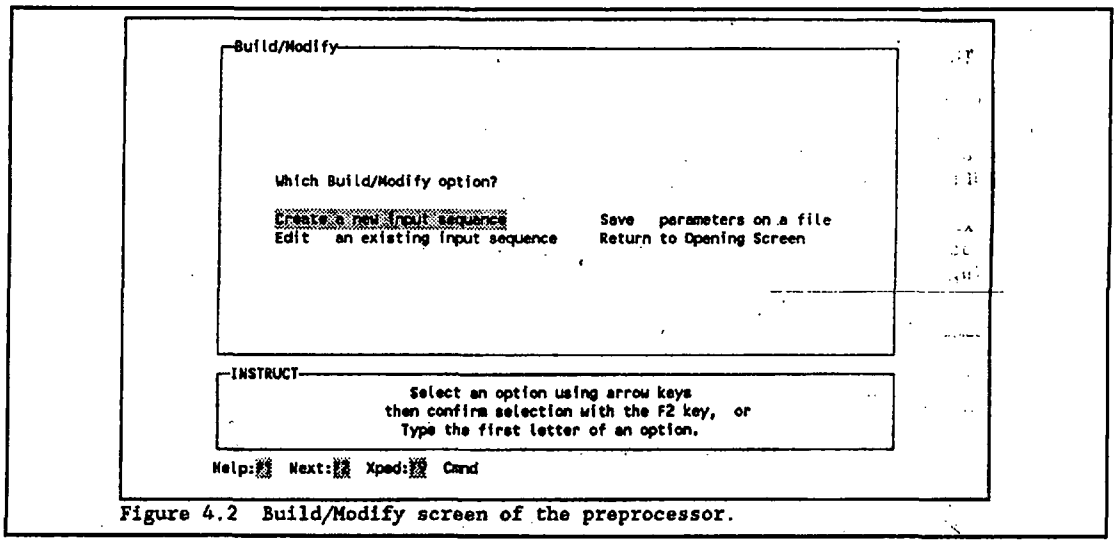


Figure 4.2 Build/Modify screen of the preprocessor.

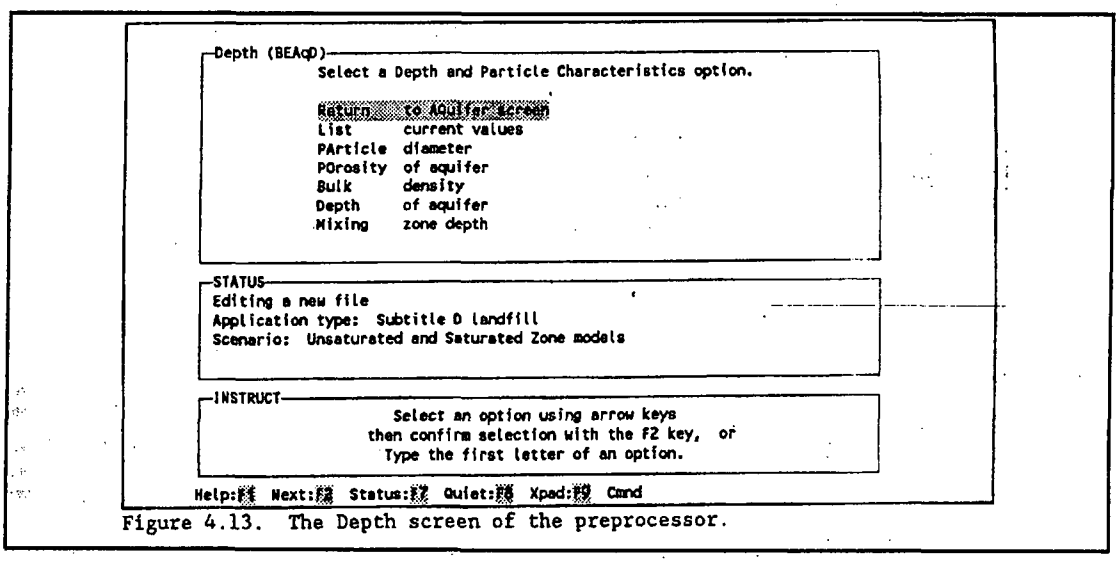


Figure 4.13. The Depth screen of the preprocessor.

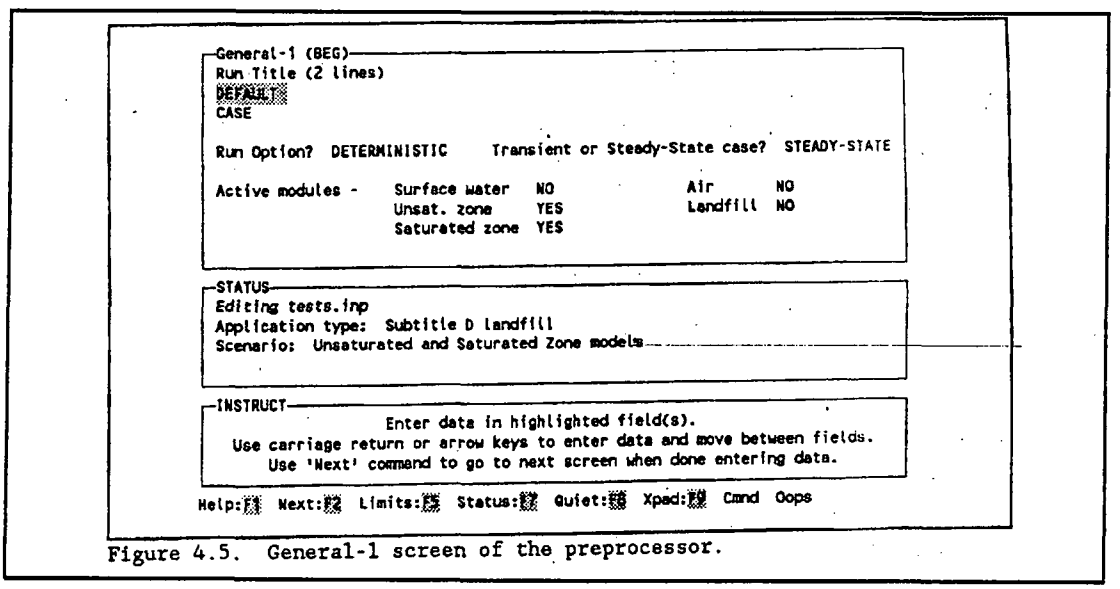


Figure 4.5. General-1 screen of the preprocessor.

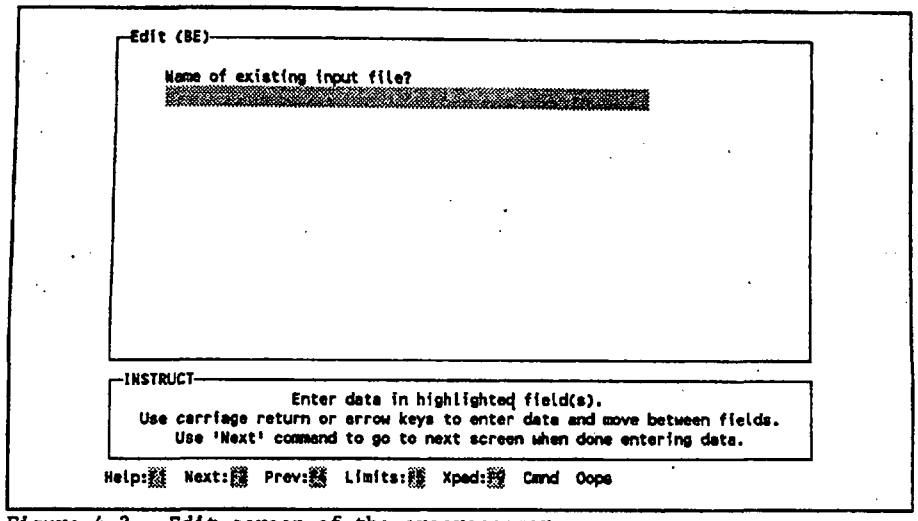


Figure 4.3. Edit screen of the preprocessor.

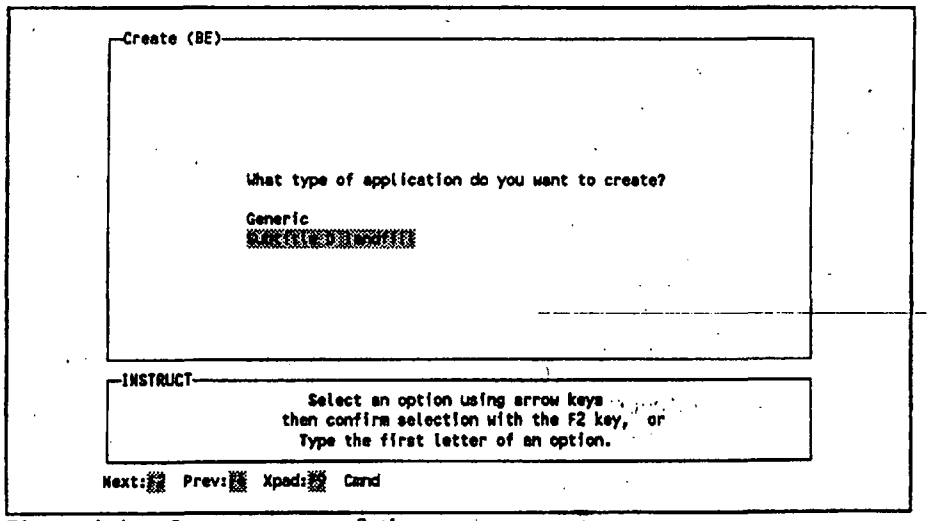


Figure 4.4. Create screen of the preprocessor.

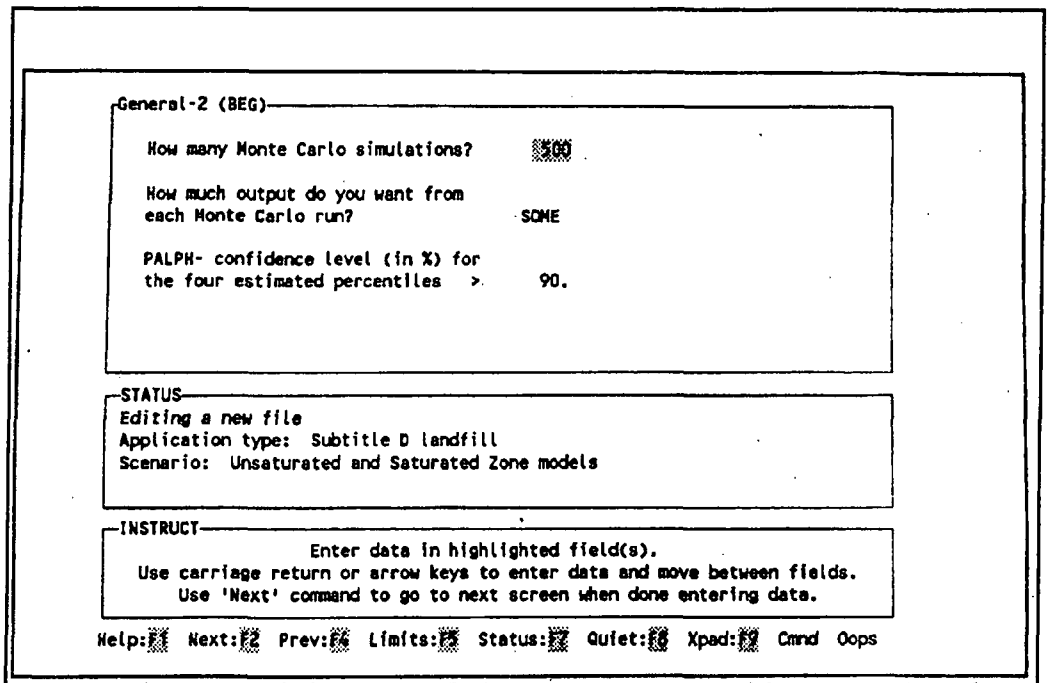


Figure 4.6. General-2 screen of the preprocessor. This screen is only activated if the simulation is run in Monte Carlo mode.

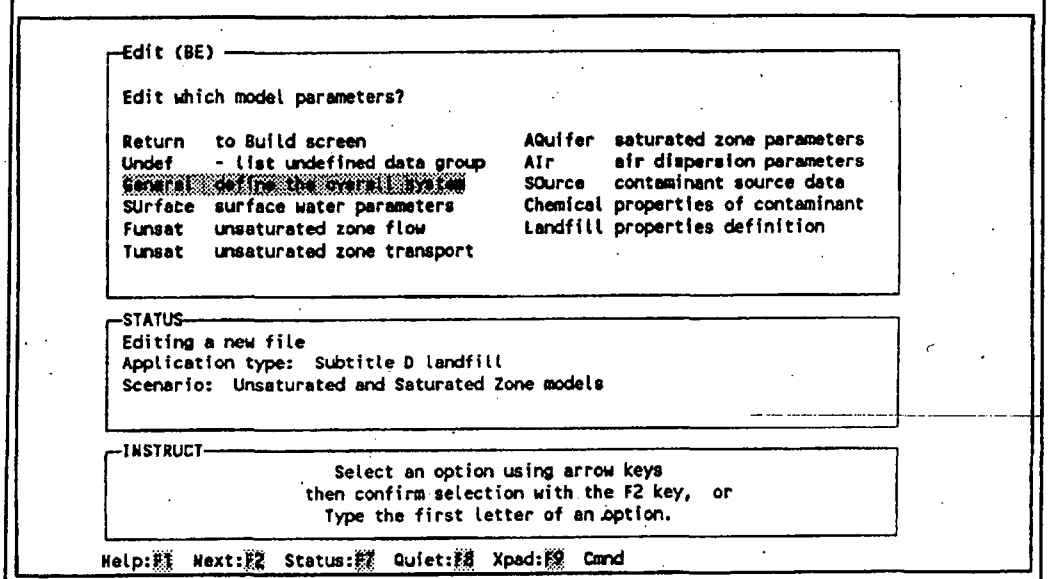


Figure 4.7. The Edit screen of the preprocessor.

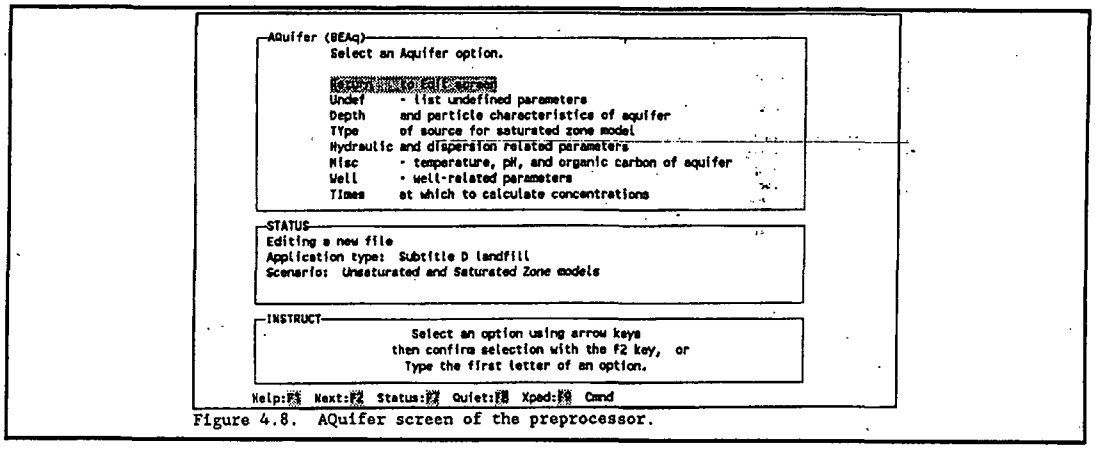


Figure 4.8. AQuifer screen of the preprocessor.

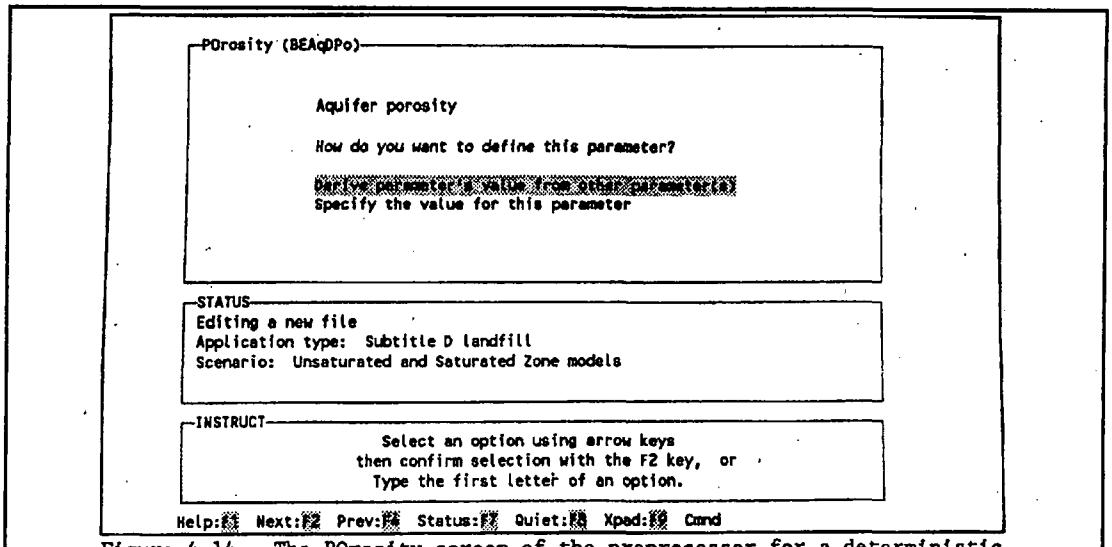


Figure 4.14. The POrosity screen of the preprocessor for a deterministic simulation.

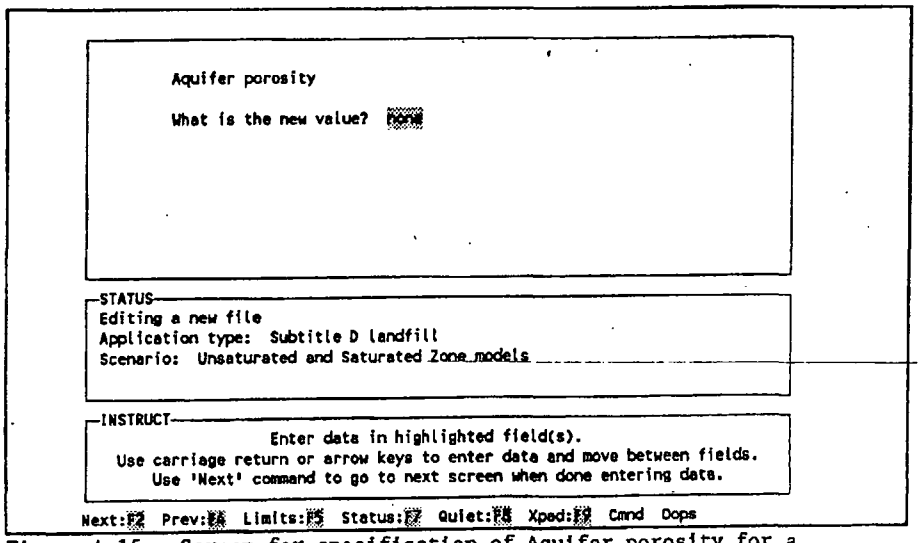


Figure 4.15. Screen for specification of Aquifer porosity for a deterministic simulation.

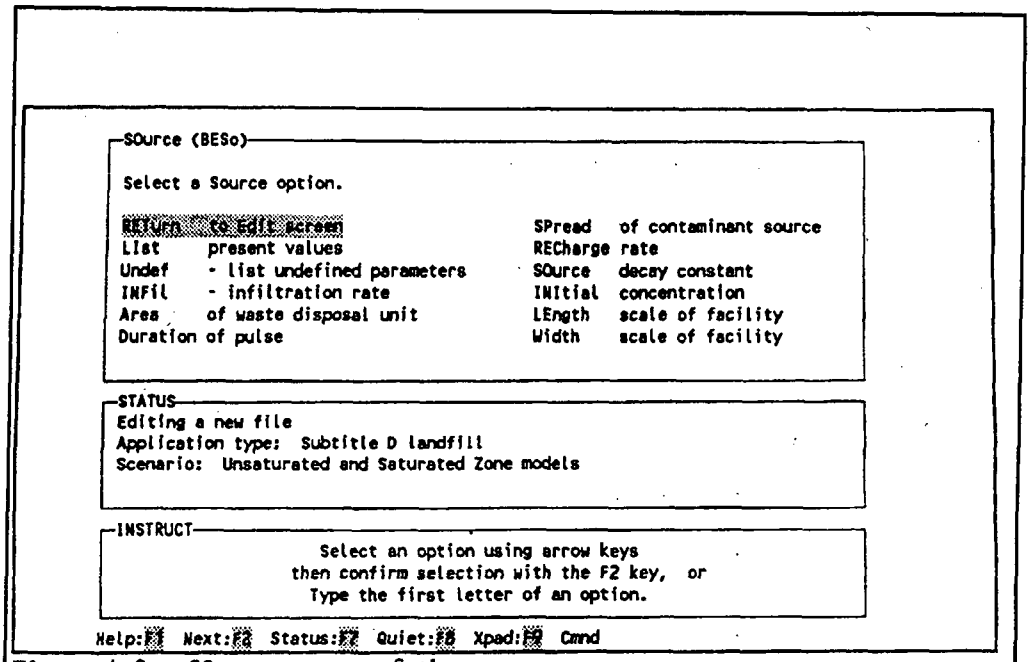


Figure 4.9. SOurce screen of the preprocessor.

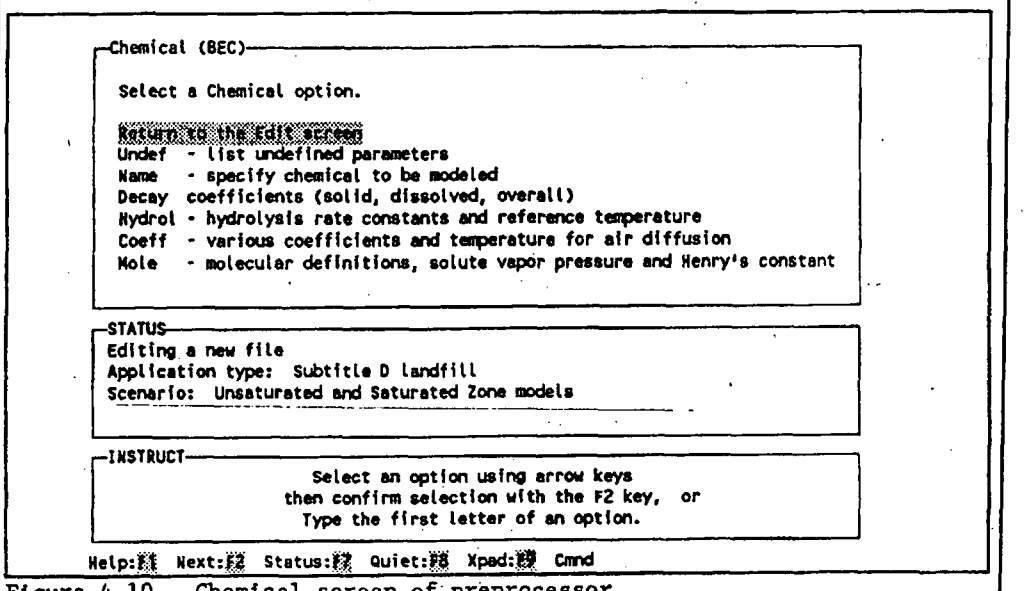


Figure 4.10. Chemical screen of preprocessor.

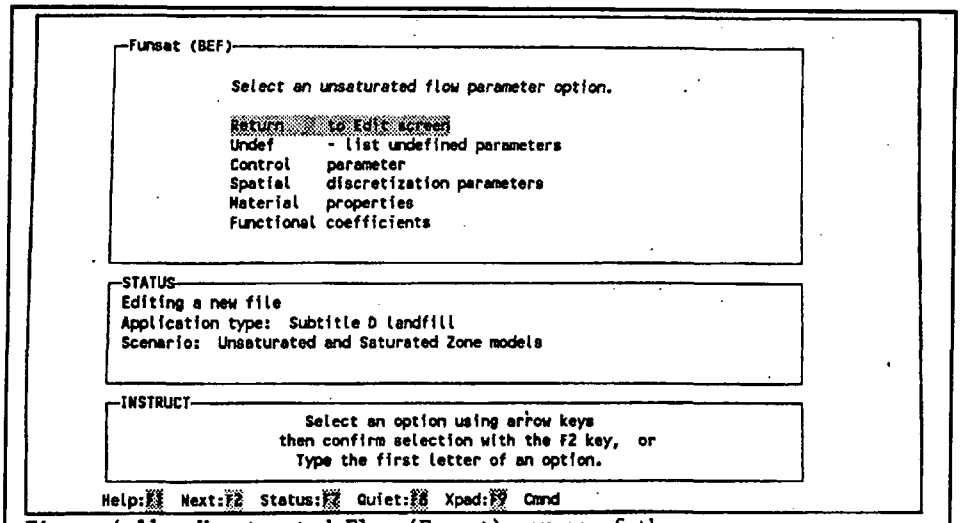


Figure 4.11. Unsaturated Flow (Funsat) screen of the preprocessor.

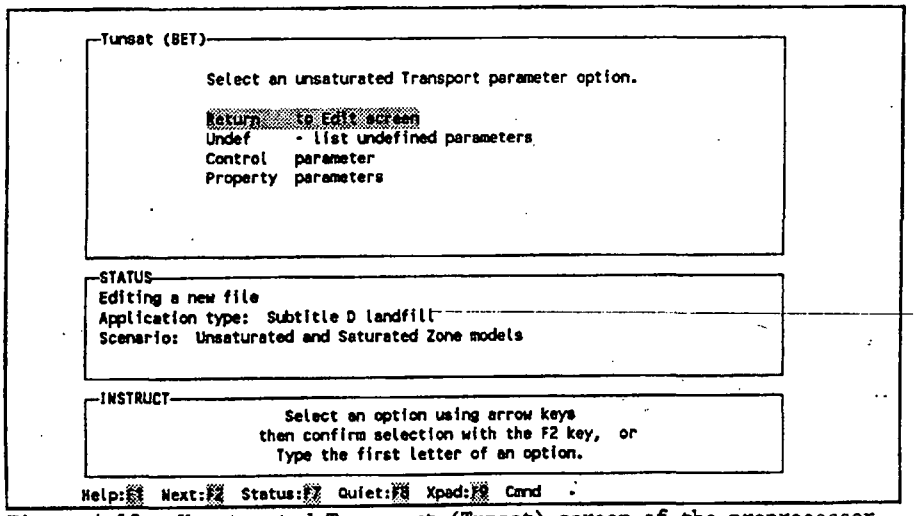


Figure 4.12. Unsaturated Transport (Tunsat) screen of the preprocessor.

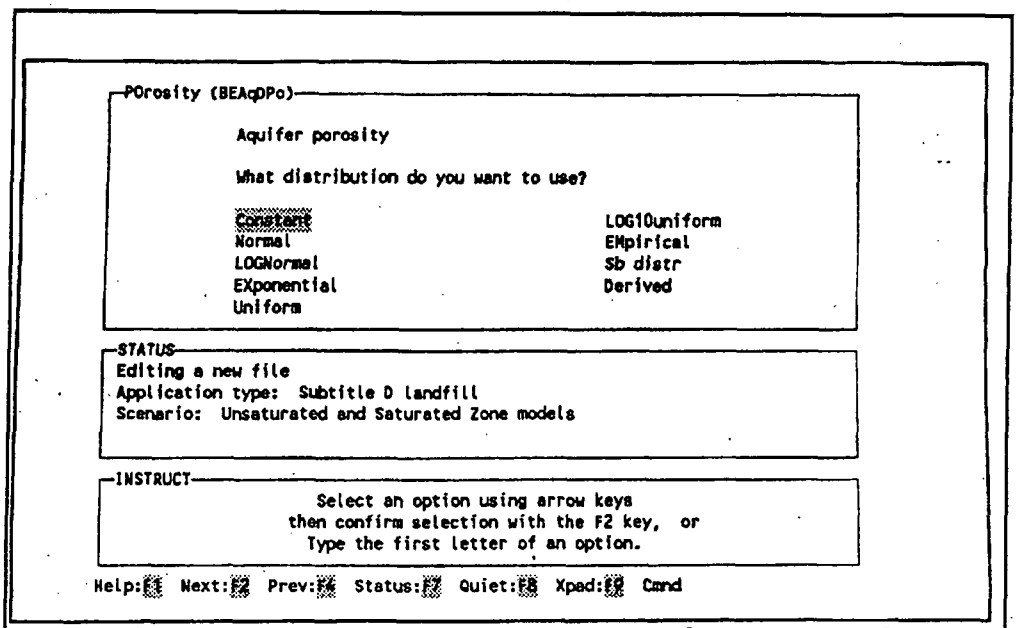


Figure 4.16. Porosity screen of the preprocessor for a Monte Carlo simulation.

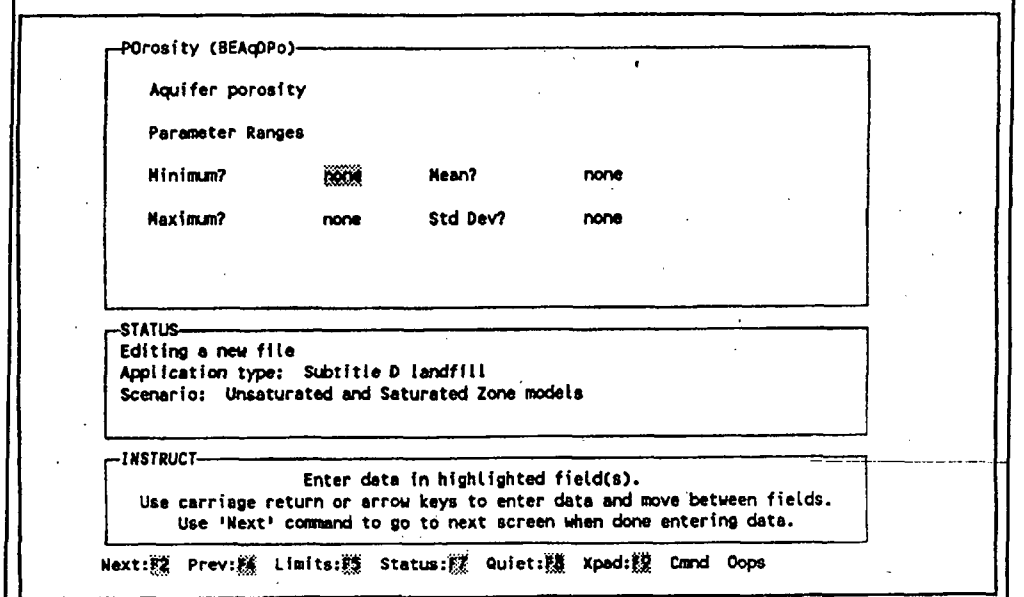


Figure 4.17. Screen showing required parameters for a Lognormal probability density distribution.

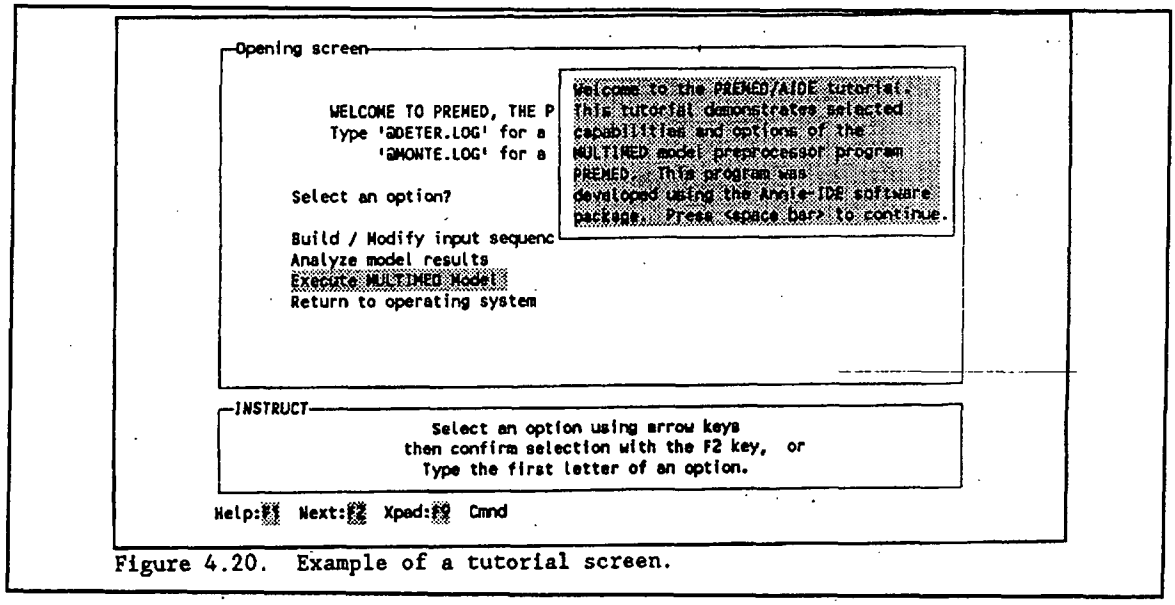


Figure 4.20. Example of a tutorial screen.

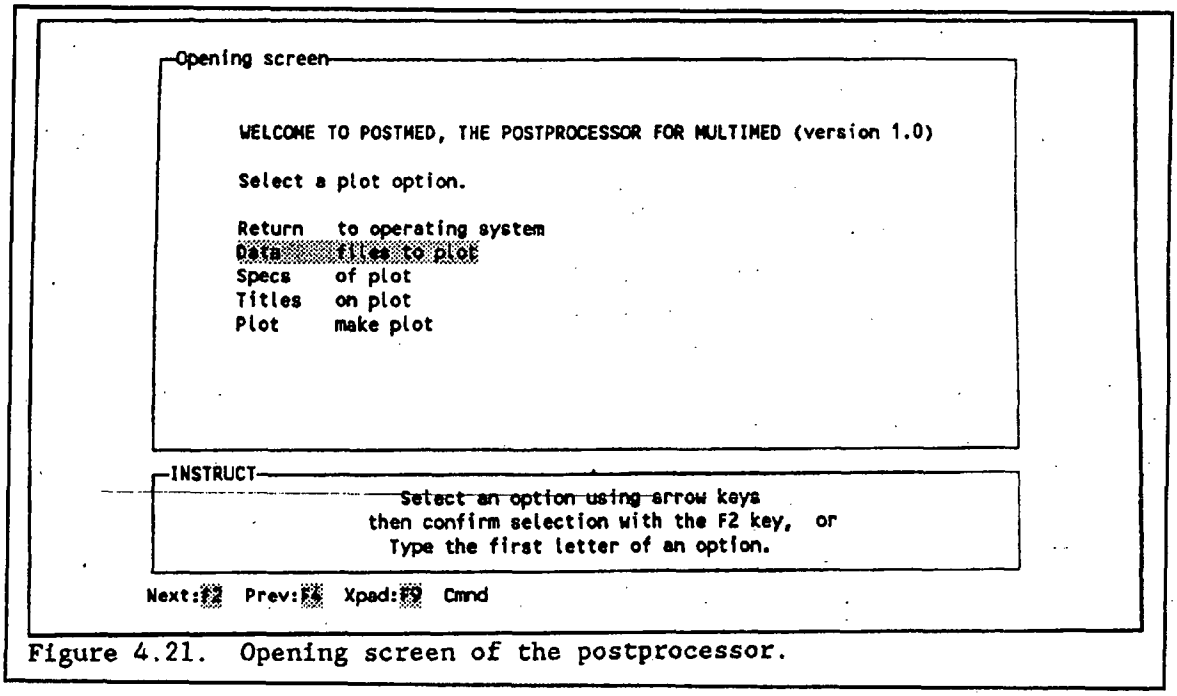


Figure 4.21. Opening screen of the postprocessor.

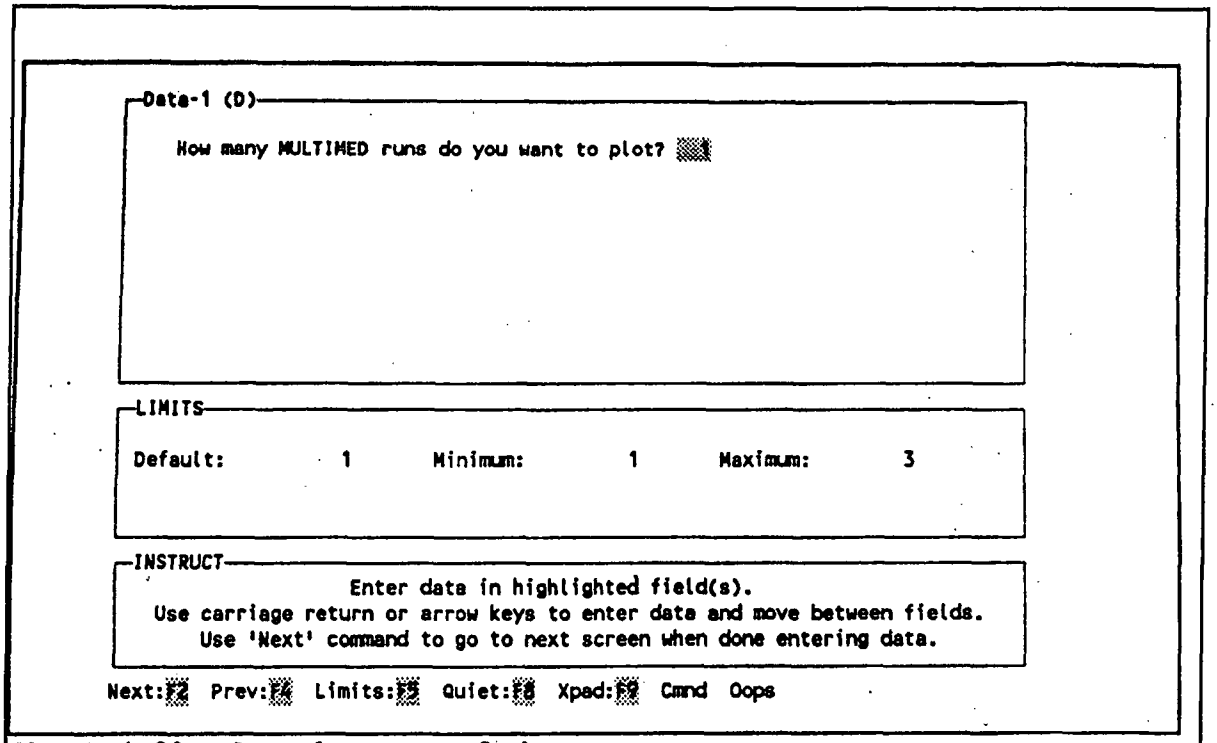


Figure 4.22. Data-1 screen of the postprocesssor.

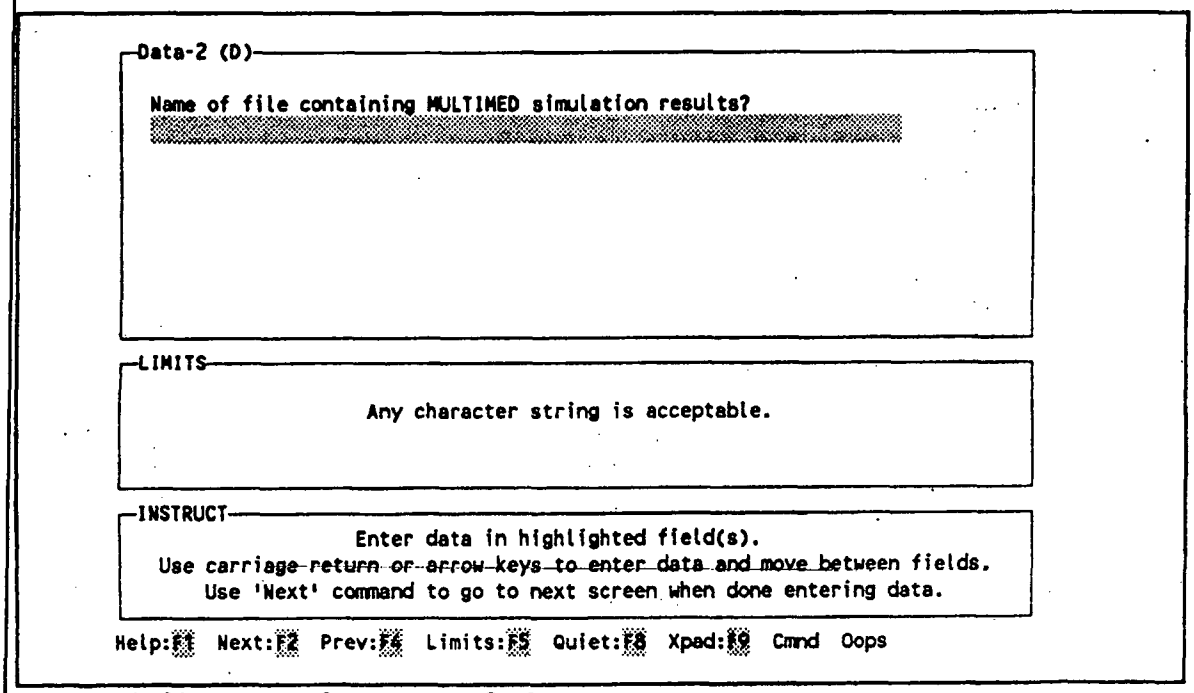


Figure 4.23. Data-2 screen of the postprocessor.

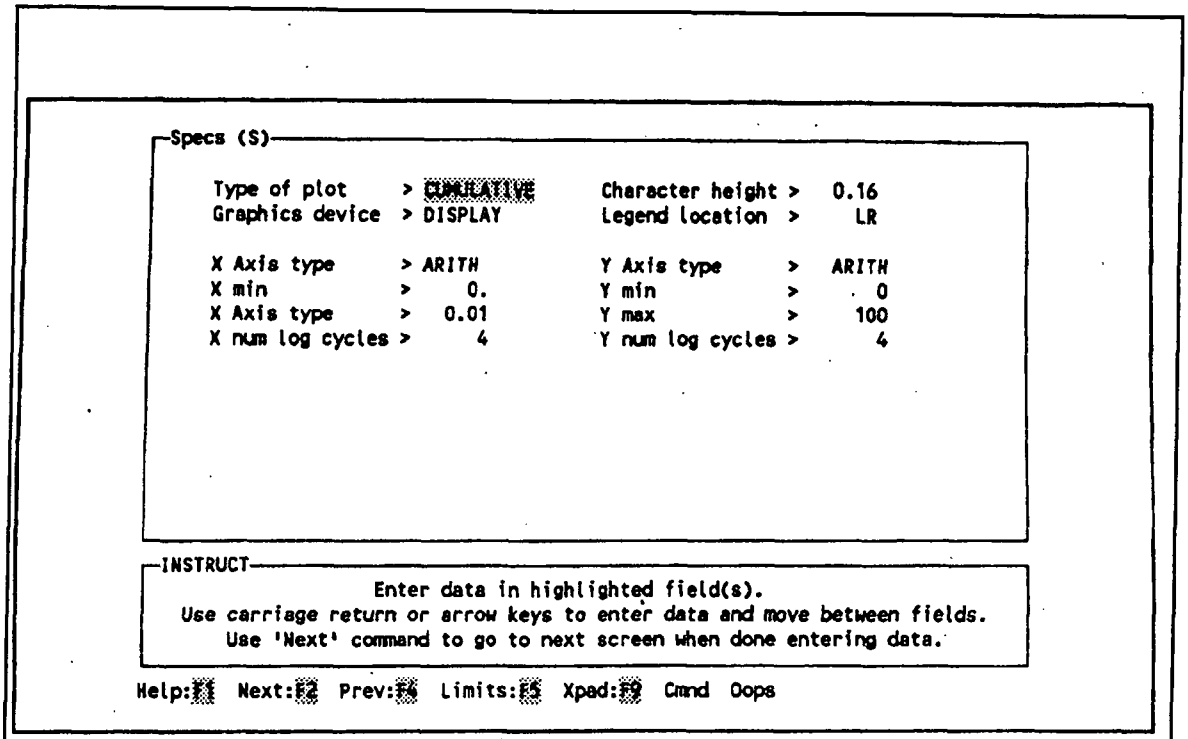


Figure 4.24. Specs screen of the postprocessor.

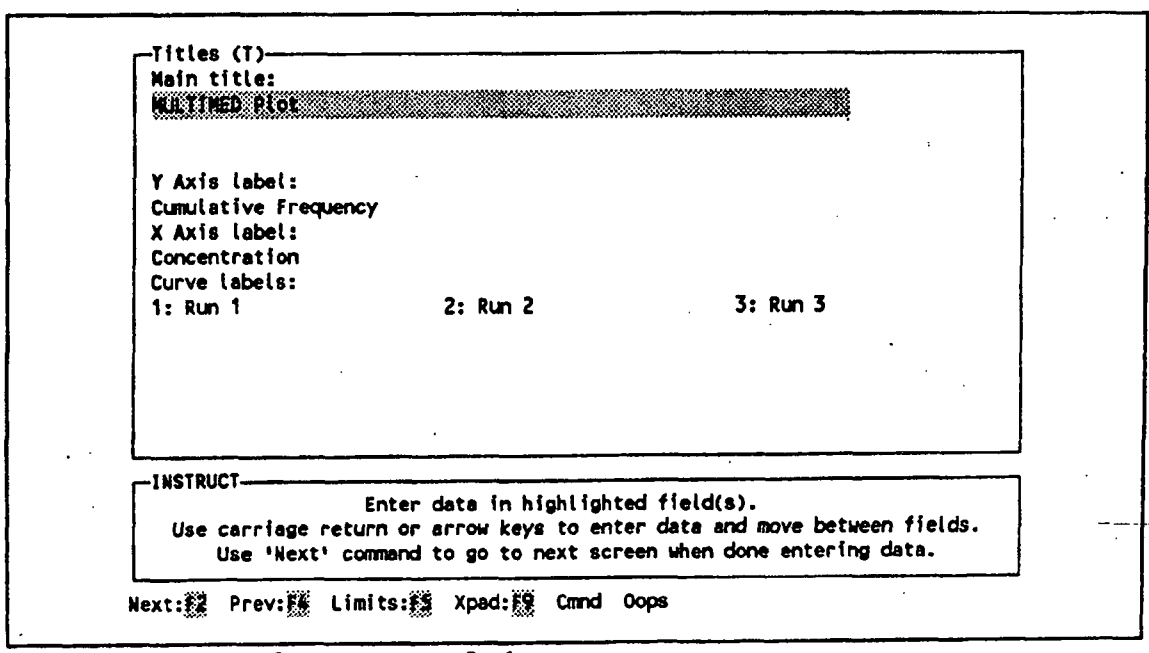
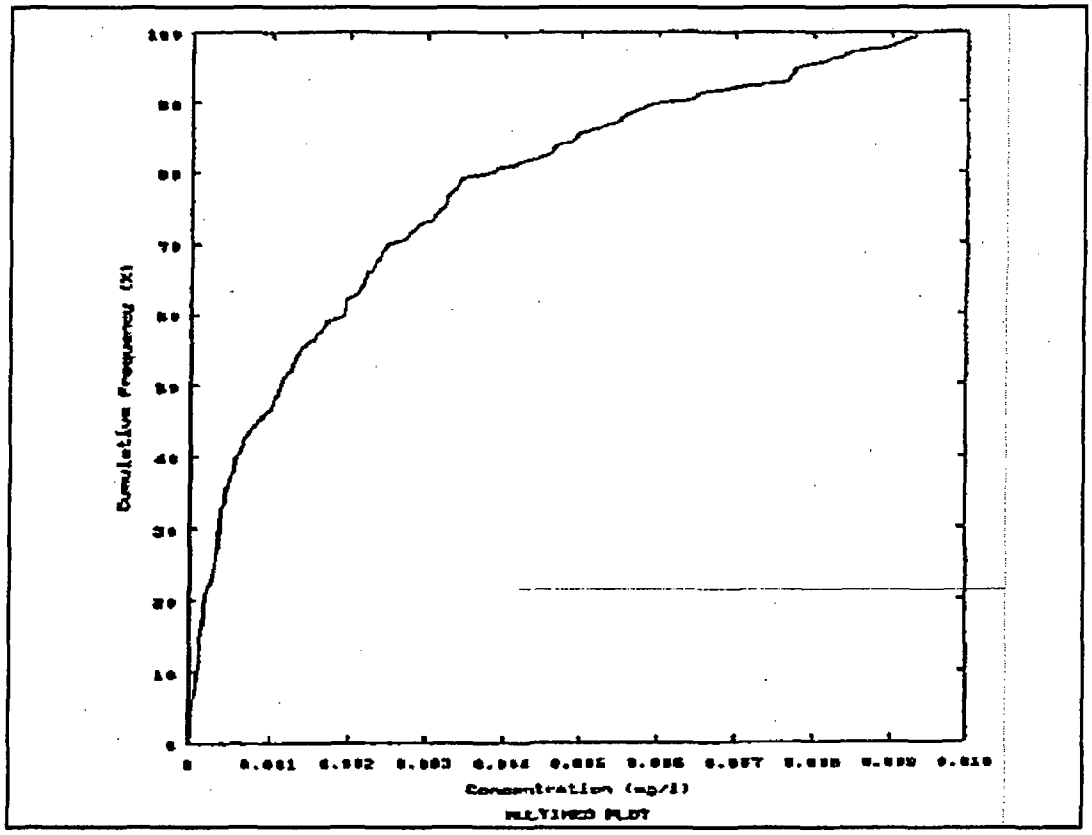
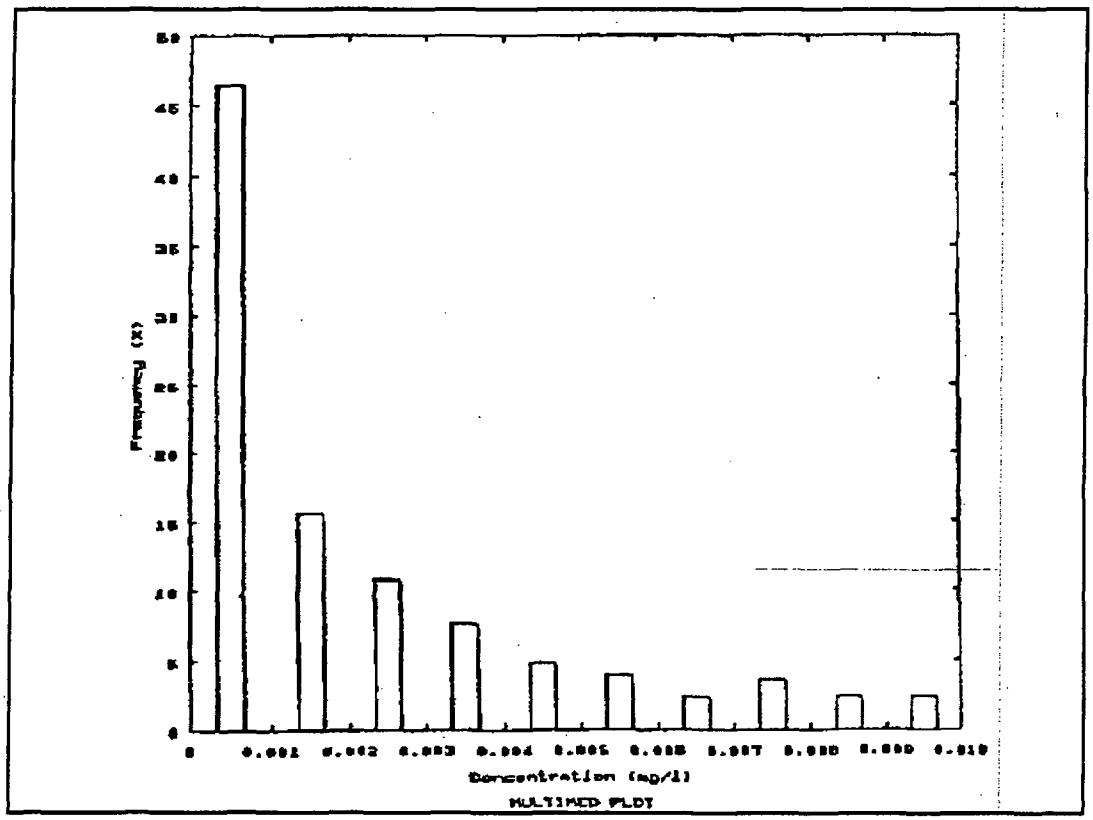


Figure 4.25. Titles screen of the postprocessor.


Cumulative Frequency (%)
Concentration (mg/l)
MULTIMED PLOT


Frequency (%)
Concentration (mg/l)
MULTIMED PLOT

Opening screen

CURVE NUMBER: 1 Run 1

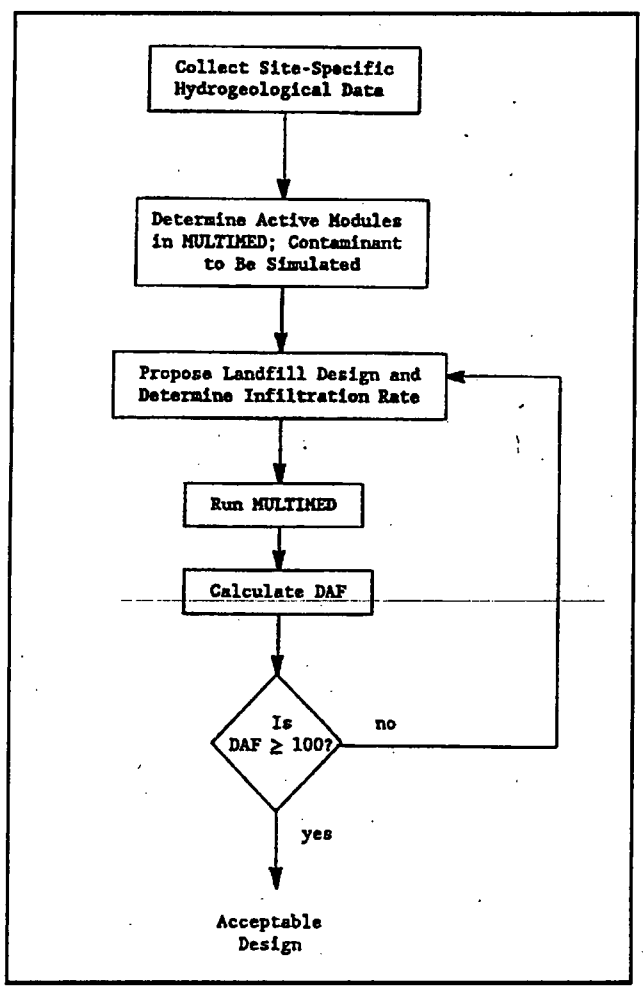
CONC	PERCENT
0.55923E-05	0.400
0.10370E-04	0.800
0.12765E-04	1.200
0.19671E-04	1.600
0.19701E-04	2.000
0.21278E-04	2.400
0.21345E-04	2.800
0.21498E-04	3.200
0.25470E-04	3.600
0.29032E-04	4.000
0.32480E-04	4.400
0.33341E-04	4.800
0.36069E-04	5.200

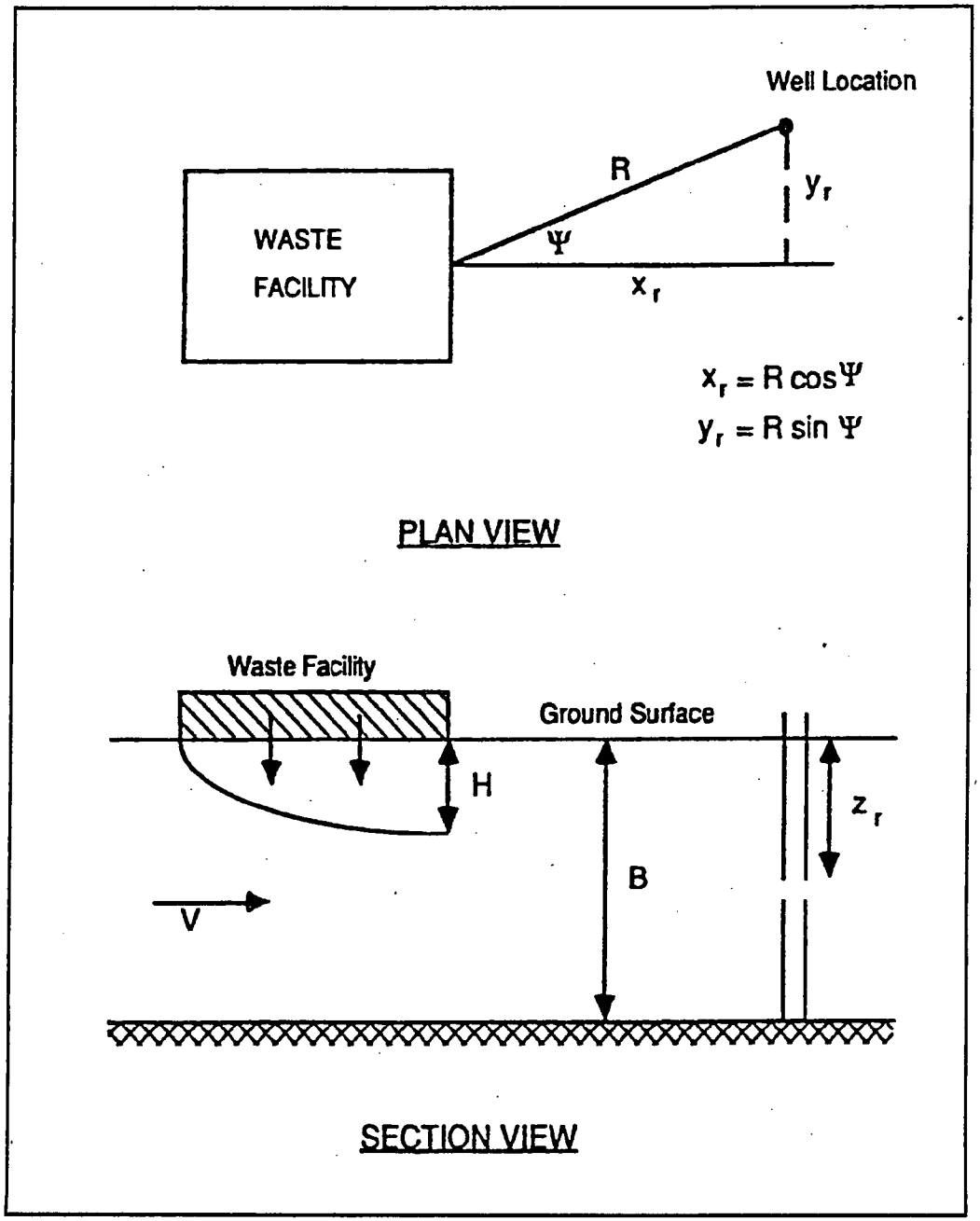
INSTRUCT

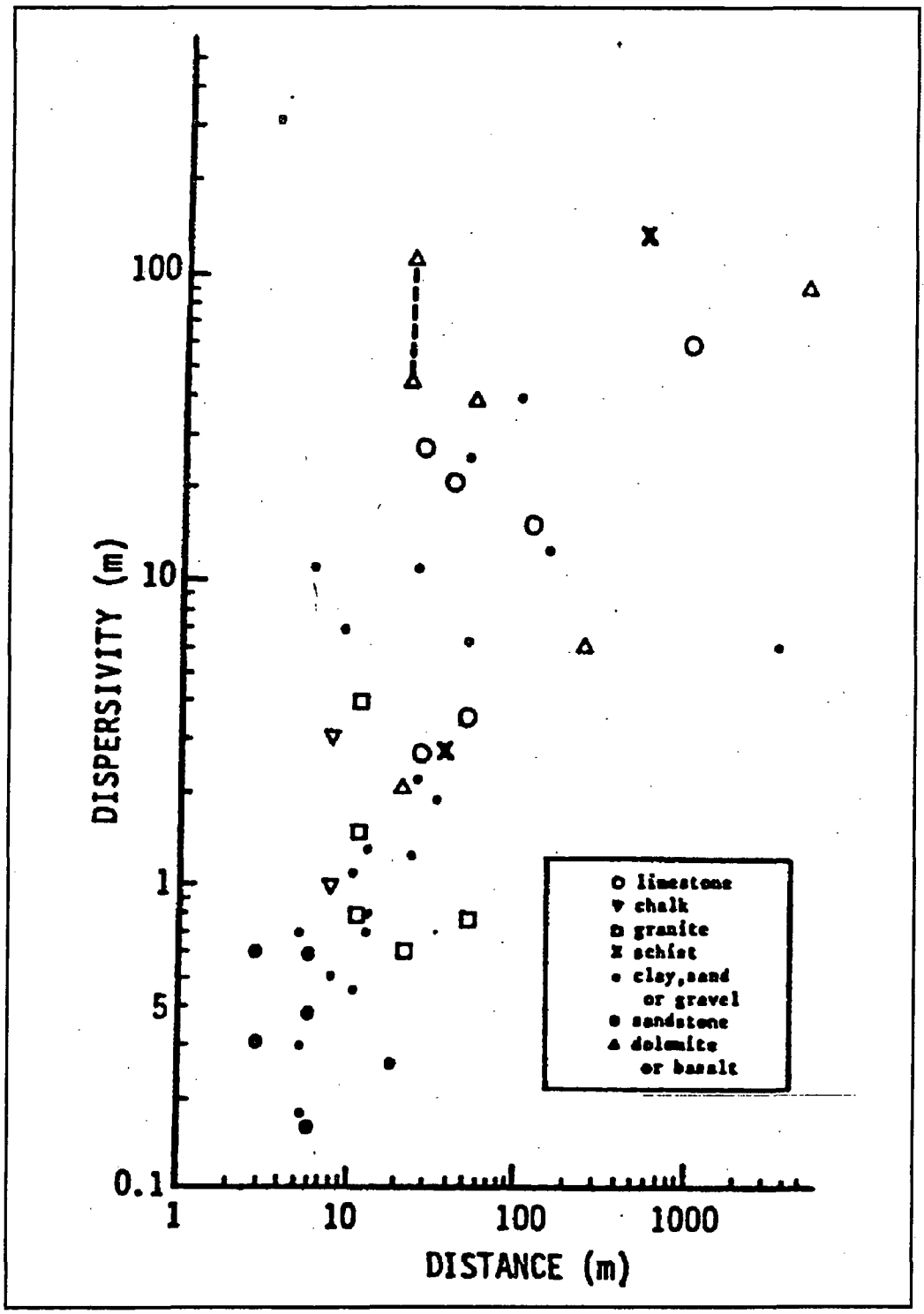
'Next' command to go to next screen

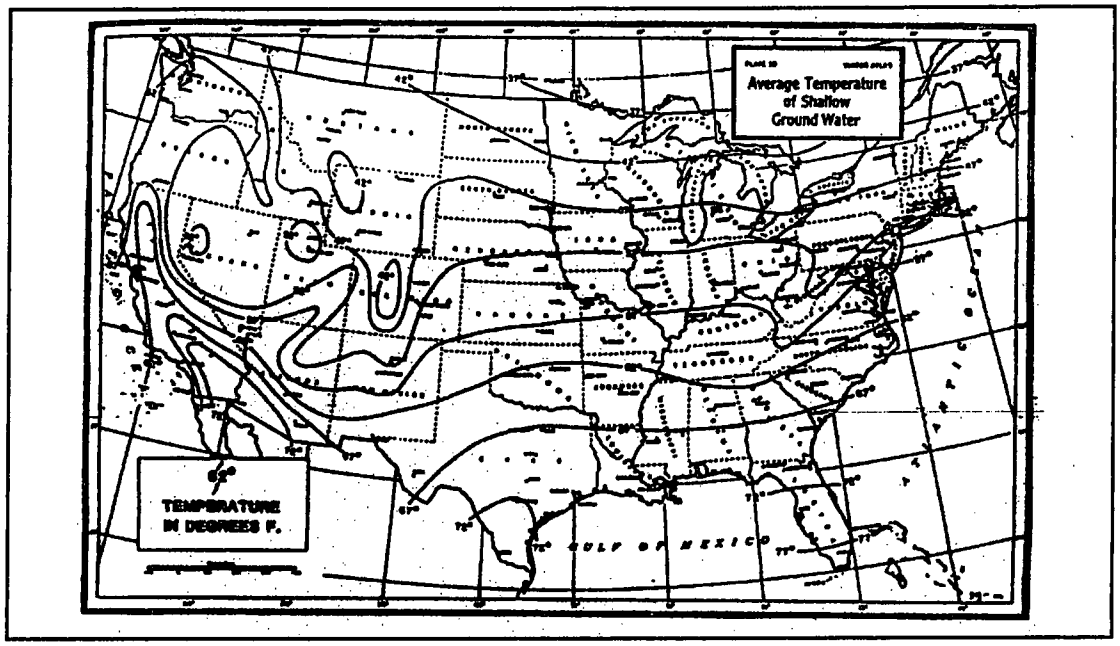
Next:F2 Prev:F4 Xpad:F9 Cmnd

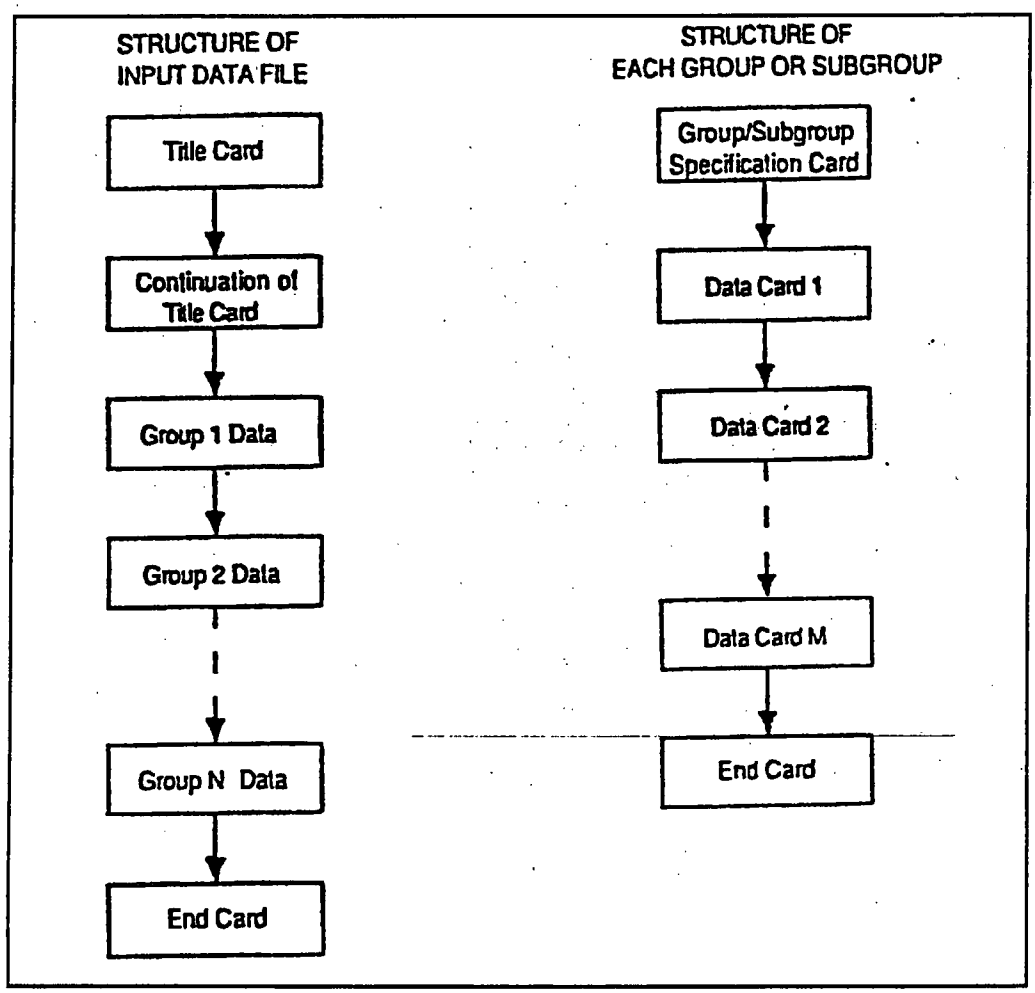
Figure 4.28. Example of screen showing a TEXT file (corresponds to cumulative frequency plot shown in Figure 4.26).

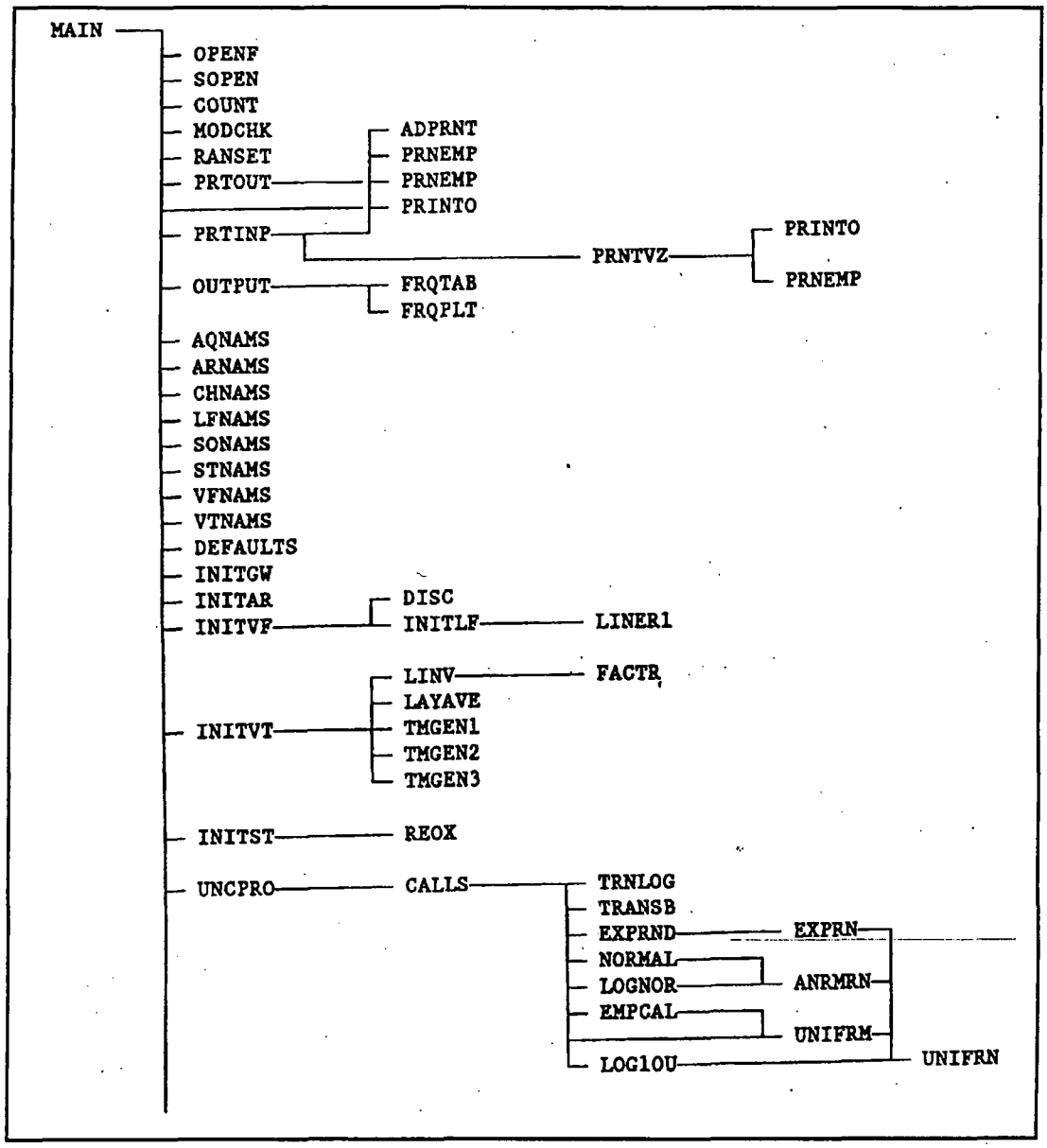


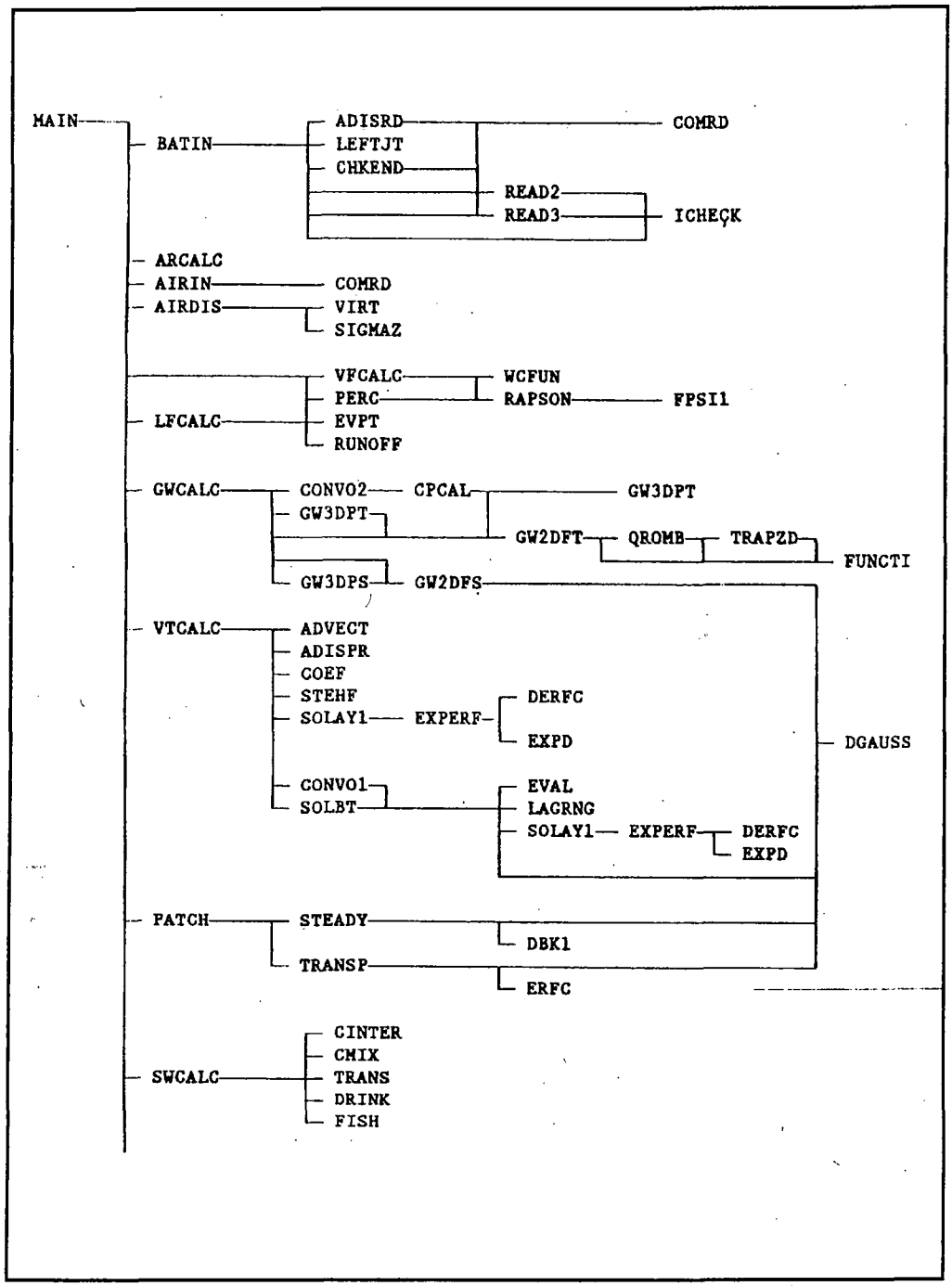

Well Location
R
y_r
WASTE
FACILITY
Ψ
x_r
$x_r = R \cos\Psi$
$y_r = R \sin\Psi$
PLAN VIEW
Waste Facility
Ground Surface
H
B
z_r
V
SECTION VIEW

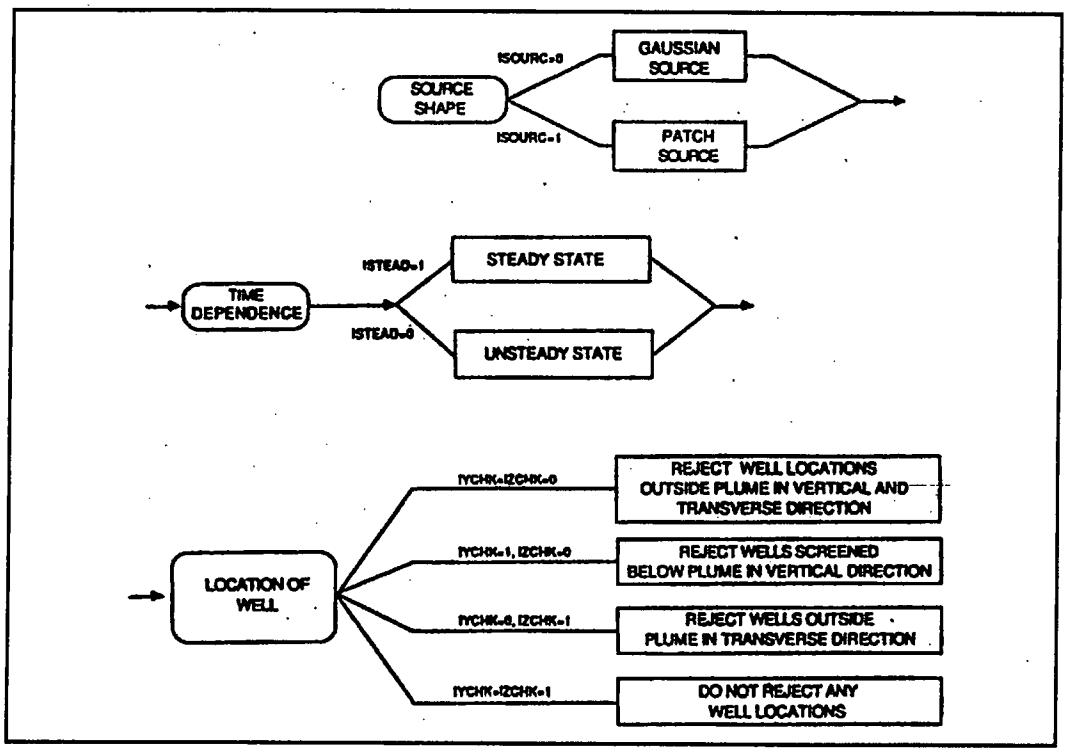

DISPERSIVITY (m)
100
10
1
5
0.1
1
10
100
1000
DISTANCE (m)
limestone
chalk
granite
schist
clay, sand or gravel
sandstone
dolomite or basalt

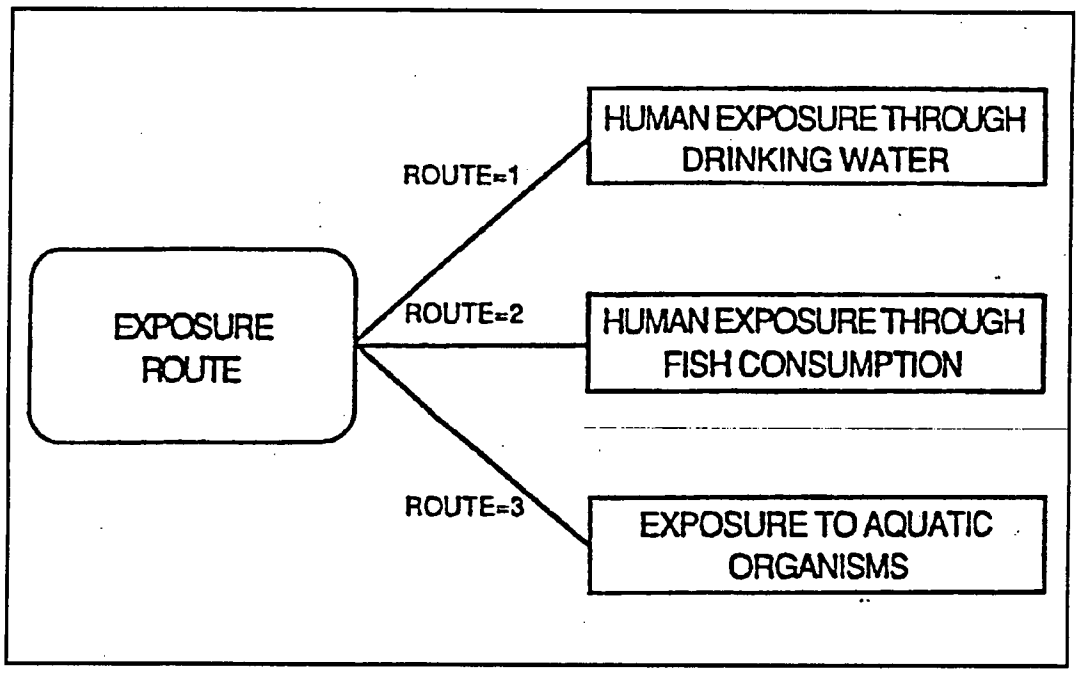

Average Temperature of Shallow Ground Water
TEMPERATURE IN DEGREES F.
GULF OF MEXICO

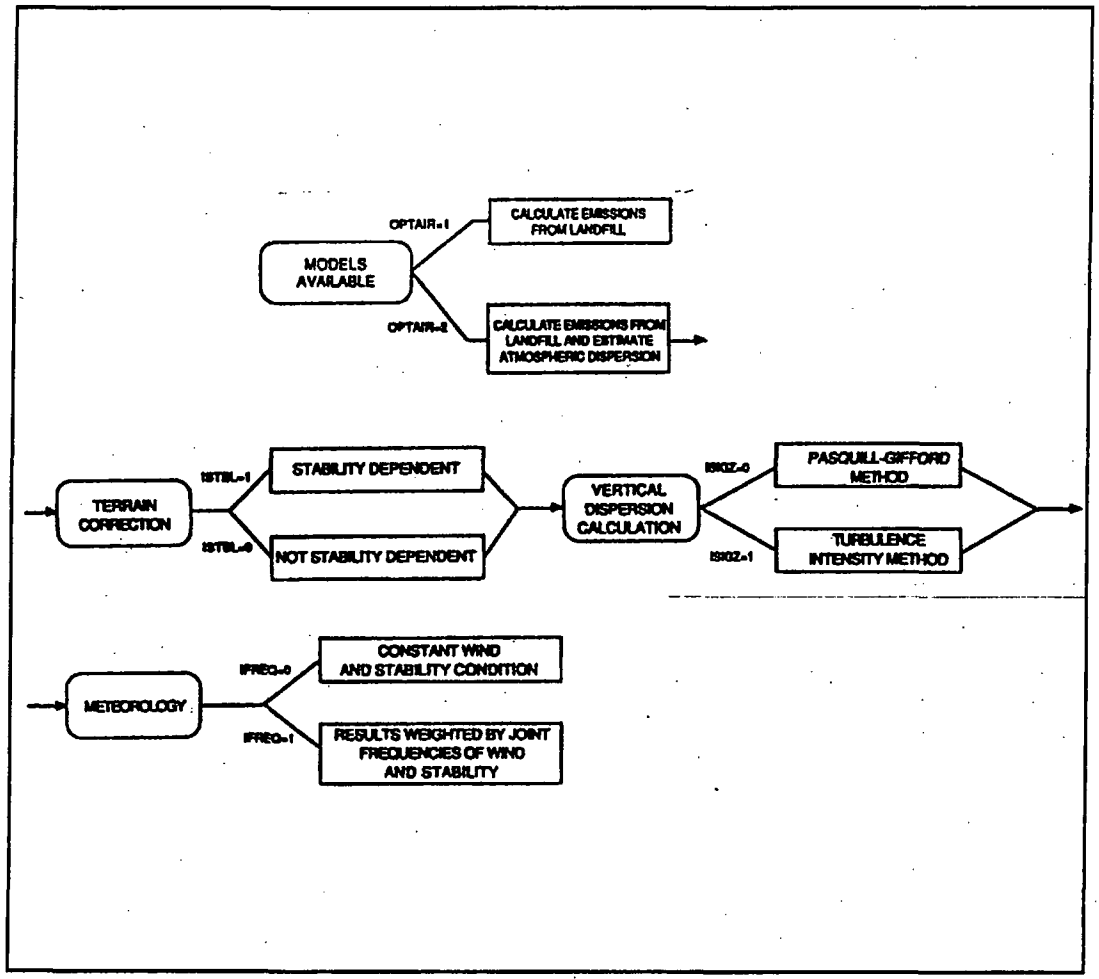

STRUCTURE OF INPUT DATA FILE
Title Card
Continuation of Title Card
Group 1 Data
Group 2 Data
Group N Data
End Card
STRUCTURE OF EACH GROUP OR SUBGROUP
Group/Subgroup Specification Card
Data Card 1
Data Card 2
Data Card M
End Card

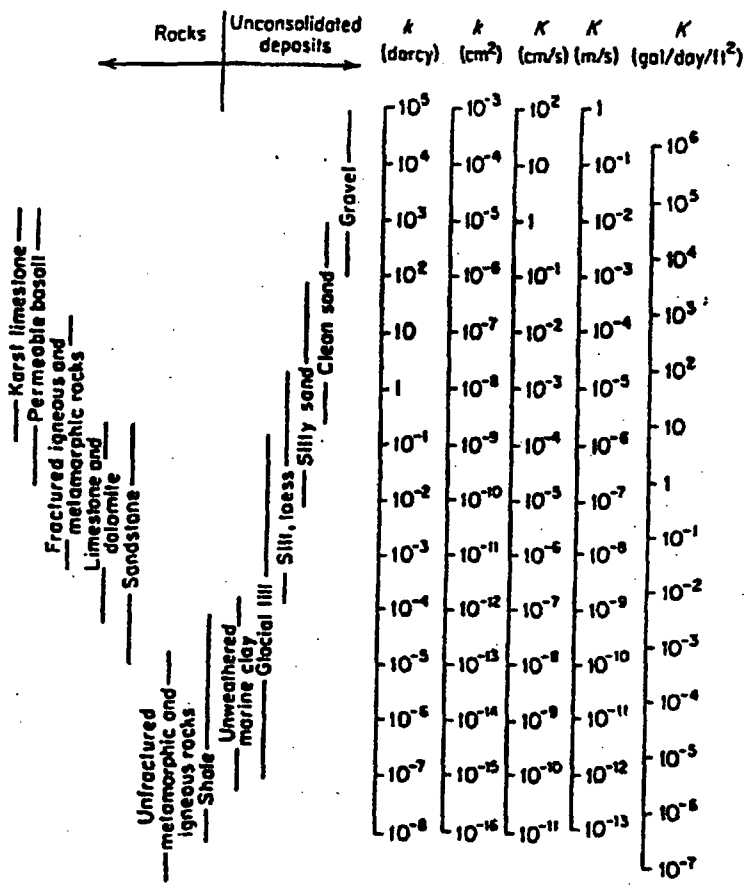

MAIN
OPENF
SOPEN
COUNT
MODCHK
RANSET
PRTOUT
ADPRNT
PRNEMP
PRNEMP
PRINTO
PRTINP
PRNTVZ
PRINTO
PRNEMP
OUTPUT
FRQTAB
FRQPLT
AQNAMS
ARNAMS
CHNAMS
LFNAMS
SONAMS
STNAMS
VFNAMS
VTNAMS
DEFAULTS
INITGW
INITAR
INITVF
DISC
INITLF
LINER1
LINV
FACTR
LAYAVE
INITVT
TMGEN1
TMGEN2
TMGEN3
INITST
REOX
UNCPRO
CALLS
TRNLOG
TRANSB
EXPRND
EXPRN
NORMAL
LOGNOR
ANRMRN
EMPCAL
UNIFRM
LOG10U
UNIFRN


MAIN
BATIN
ADISRD
LEFTJT
CHKEND
READ2
READ3
COMRD
ICHECK
ARCALC
AIRIN
COMRD
AIRDIS
VIRT
SIGMAZ
LFCALC
VFCALC
PERC
EVPT
RUNOFF
WCFUN
RAPSON
FPSI1
GWCALC
CONVO2
CPCAL
GW3DPT
GW3DPT
GW2DFT
QROMB
TRAPZD
FUNCTI
GW3DPS
GW2DFS
VTCALC
ADVECT
ADISPR
COEF
STEHF
SOLAY1
EXPERF
DERFC
EXPD
DGAUSS
CONVO1
SOLBT
EVAL
LAGRNG
SOLAY1
EXPERF
DERFC
EXPD
PATCH
STEADY
DBK1
TRANSP
ERFC
SWCALC
CINTER
CMIX
TRANS
DRINK
FISH


SOURCE SHAPE
ISOURC=0
GAUSSIAN SOURCE
ISOURC=1
PATCH SOURCE
TIME DEPENDENCE
ISTEAD=1
STEADY STATE
ISTEAD=0
UNSTEADY STATE
LOCATION OF WELL
IYCHK=I2CHK=0
REJECT WELL LOCATIONS OUTSIDE PLUME IN VERTICAL AND TRANSVERSE DIRECTION
IYCHK=1, I2CHK=0
REJECT WELLS SCREENED BELOW PLUME IN VERTICAL DIRECTION
IYCHK=0, I2CHK=1
REJECT WELLS OUTSIDE PLUME IN TRANSVERSE DIRECTION
IYCHK=I2CHK=1
DO NOT REJECT ANY WELL LOCATIONS


EXPOSURE ROUTE
ROUTE=1
HUMAN EXPOSURE THROUGH DRINKING WATER
ROUTE=2
HUMAN EXPOSURE THROUGH FISH CONSUMPTION
ROUTE=3
EXPOSURE TO AQUATIC ORGANISMS


MODELS AVAILABLE
OPTAIR=1
CALCULATE EMISSIONS FROM LANDFILL
OPTAIR=2
CALCULATE EMISSIONS FROM LANDFILL AND ESTIMATE ATMOSPHERIC DISPERSION
TERRAIN CORRECTION
ISTBL=1
STABILITY DEPENDENT
ISTBL=0
NOT STABILITY DEPENDENT
VERTICAL DISPERSION CALCULATION
ISIGZ=0
PASQUILL-GIFFORD METHOD
ISIGZ=1
TURBULENCE INTENSITY METHOD
METEOROLOGY
IFREQ=0
CONSTANT WIND AND STABILITY CONDITION
IFREQ=1
RESULTS WEIGHTED BY JOINT FREQUENCIES OF WIND AND STABILITY



Conversion Factors for Permeability and Hydraulic Conductivity Units

	Permeability, k*			Hydraulic conductivity, K		
	cm^2	ft^2	darcy	m/s	ft/s	U.S. gal/day/ft^2
cm^2	1	1.08×10^{-3}	1.01×10^{8}	9.80×10^{2}	3.22×10^{3}	1.85×10^{9}
ft^2	9.29×10^{2}	1	9.42×10^{10}	9.11×10^{5}	2.99×10^{6}	1.71×10^{12}
darcy	9.87×10^{-9}	1.06×10^{-11}	1	9.66×10^{-6}	3.17×10^{-5}	1.82×10^{1}
m/s	1.02×10^{-3}	1.10×10^{-6}	1.04×10^{5}	1	3.28	2.12×10^{6}
ft/s	3.11×10^{-4}	3.35×10^{-7}	3.15×10^{4}	3.05×10^{-1}	1	6.46×10^{5}
U.S. gal/day/ft^2	5.42×10^{-10}	5.83×10^{-13}	5.49×10^{-2}	4.72×10^{-7}	1.55×10^{-6}	1

*To obtain k in ft^2, multiply k in cm^2 by 1.08×10^{-3}.