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Superfund Exposure Assessment Manual

U.S. Environmental Protection Agency
Office of Remedial Response
Washington, DC 20460

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Table of Contents

Chapter **Page**

List of Tables vi
List of Figures viii
Foreword ix
Executive Summary xi
Acknowledgments xii

1 INTRODUCTION 1

1.1 Purpose 1
1.2 Background 1
1.3 Scope 1
1.4 Use of the Manual 2
1.5 Timeframe of Analysis 4
1.6 Analysis of Exposure Associated with Remedial Actions 4
1.7 Organization of the Manual 5

2 CONTAMINANT RELEASE ANALYSIS 7

2.1 Introduction 7
2.2 Contaminant Release Screening 8
2.2.1 Contaminants in Soil 8
2.2.2 Contaminants Above-Ground 10
2.3 Quantitative Analysis of Atmospheric Contamination 10
2.3.1 Fugitive Dust Emission Analysis 10
2.3.1.1 Beginning Quantitative Analysis 10
2.3.1.2 In-Depth Analysis 14
2.3.2 Volatilization Emission Analysis 14
2.3.2.1 Beginning Quantitative Analysis 14
2.3.2.2 In-Depth Analysis 21
2.3.3 Long-Term and Short-Term Release Calculation 22
2.4 Quantitative Analysis of Surface Water Contamination 22
2.4.1 Beginning Quantitative Analysis 23
2.4.1.1 Dissolved and Sorbed Contaminant Migration 23
2.4.2 In-Depth Analysis 25
2.4.3 Long-Term and Short-Term Release Calculation 27
2.5 Quantitative Analysis of Ground-Water Contamination 29
2.5.1 Beginning Quantitative Analysis 29
2.5.1.1 Leachate Release Rate 29
2.5.2 In-Depth Analysis 31
2.5.3 Long-Term and Short-Term Release Calculation 31
2.6 Soil Contamination 31
2.6.1 Beginning Quantitative Analysis 31
2.6.2 In-Depth Analysis 31

3 CONTAMINANT FATE ANALYSIS 35

3.1 Introduction 35
3.2 Contaminant Fate Screening 36

Table of Contents (Continued)

Chapter		Page
	3.2.1 Atmospheric Fate	36
	3.2.2 Surface Water Fate	38
	3.2.3 Soil and Ground-Water Fate	40
	3.2.4 Biotic Fate	40
3.3	Quantitative Analysis of Atmospheric Fate	42
	3.3.1 Screening Analysis	42
	3.3.2 In-Depth Analysis.	46
	3.3.2.1 Intermedia Transfer	46
	3.3.2.2 Intramedia Transformation Processes	47
	3.3.2.3 The Effects of Terrain	48
	3.3.3 Computer Models	48
	3.3.4 Short- and Long-Term Concentration Calculations	48
3.4	Surface Water Fate Analysis	53
	3.4.1 Beginning Quantitative Analysis	53
	3.4.2 In-Depth Analysis.	55
	3.4.2.1 Intermedia Transfers	55
	3.4.2.2 Intramedia Transformation Processes	56
	3.4.2.3 Computer Models	56
	3.4.2.4 Short- and Long-Term Concentration Calculations	57
3.5	Quantitative Analysis of Ground-Water Fate	57
	3.5.1 Discussion of Ground Water Modeling	63
	3.5.1.1 The Contamination Cycle	63
	3.5.1.2 Ground Water Flow Conditions	64
	3.5.1.3 Multiphase Flow	65
	3.5.1.4 Contaminant Flow and Hydrodynamic Dispersion	65
	3.5.1.5 Transformation and Retardation	66
	3.5.1.6 Higher Velocity Transport	68
	3.5.2 Ground-Water Modeling Equations and Nomograph	68
	3.5.2.1 Calculating Ground Water Velocity	68
	3.5.2.2 Calculating the Velocity of Infiltrating Rainwater	69
	3.5.2.3 Corrections for Viscosity and Density	73
	3.5.2.4 Retardation Effects	73
	3.5.2.5 Contaminant Velocity	75
	3.5.2.6 Nomograph Technique	77
	3.5.2.7 Extent of Plume	77
	3.5.2.8 Use of Monitoring Data	82
	3.5.2.9 VHS Model	82
	3.5.3 In-Depth Methods and Models	83
	3.5.4 Short- and Long-Term Concentration Calculations	93
3.6	Biotic Pathways	93
	3.6.1 Estimation Procedures	93
	3.6.1.1 Aquatic Animals..	94
	3.6.1.2 Terrestrial Animals	94
	3.6.1.3 Terrestrial Plants	94
4	UNCERTAINTY IN THE ANALYSIS	95
4.1	Sources of Uncertainty	95
	4.1.1 Input Variable Uncertainty	95
4.2	Modeling Uncertainty	96
	4.2.1 Model Simplification	96
	4.2.2 Averaging Hydraulic Conductivities	96
	4.2.3 Dispersion Simulation.	97
	4.2.4 Numerical Models and Analytical Models	97
	4.2.5 Chemical Degradation Simulation	97
	4.2.6 Model Operational Parameters	97

Table of Contents (Continued)

Chapter		Page
	4.2.7 Source Shape	98
	4.2.8 Steady State Modeling.	98
	4.2.9 Number of Dimensions Addressed by the Model	98
	4.3 Scenario Uncertainty	98
	4.4 Approaches for Dealing with Uncertainty	98
	4.4.1 Sensitivity Appraisals	98
	4.4.2 Monte-Carlo Simulations	99
	4.4.3 Using Monitoring Data to Calibrate the Model	99
	4.5 Level of Uncertainty Appropriate for Exposure Modeling	100
	4.6 Risk Communication	100
5	REFERENCES	103
APPENDIX A	Analysis of Exposed Human Populations and Exposure Calculation and Integration	113
APPENDIX B	Possible Exposure Assessment Data Requirements for Uncontrolled Hazardous Waste Sites and Index to Variable Terms	135
APPENDIX C	Data Management Forms	145

List of Tables

Number		Page
1-1	Technical Resource Contacts for Superfund Exposure Assessments	5
2-1	Potential Contaminant Release Mechanisms	8
2-2	Environmental Variables and Model Parameters for the Wind Erosion Equation	13
2-3	Diffusion Coefficients of Selected Organic Compounds	18
2-4	"C" Values for Permanent Pasture, Rangeland, and Idle Land	26
2-5	"C" Values for Woodland	26
2-6	Runoff Curve Numbers	27
2-7	Parameter Values for Permeation Equation (at 25°C)	32
2-8	Polymer Categorization for Permeation of Water	32
2-9	Permachor Values of Some Organic Liquids in Polyethylene and PVC	32
2-10	Water Permachor Value for Dry Polymers	33
3-1	Key to Stability Categories	45
3-2	Resource Requirements and Information Sources: Atmospheric Fate Models.	49
3-3	Features of Atmospheric Fate Models	51
3-4	Data Requirements for Atmospheric Models	52
3-5	Resource Requirements and Information Sources: Surface Water Fate Models	58
3-6	Feature of Surface Water Fate Models	61
3-7	Data Requirements for Surface Water Models	62
3-8	Representative Values of Saturated Hydraulic Conductivity	70
3-9	Saturated Hydraulic Conductivity Ranges for Selected Rock and Soil Types	70
3-10	Representative Values for Saturated Moisture Contents and Field Capacities of Various Soil Types	70
3-11	Representative Values of Hydraulic Parameters (Standard Deviation in Parentheses)	71
3-12	Suggested Value for C_{et} Relating Evaporation from a US Class A Pan to Evapotranspiration from 8 to 15-cm Tall, Well-watered Grass Turf	72
3-13	Crop Coefficients for Estimating Evapotranspiration	73
3-14	Resource Requirements and Information Sources: Unsaturated Zone and Ground-Water Fate Models	84
3-15	Features of Unsaturated Zone and Ground-Water Fate Models	88
3-16	Data Requirements for Unsaturated Zone and Ground-water Models	91

List of Tables (Continued)

Number		Page
A-1	Regional Census Bureau Offices	118
A-2	U.S. Home Fruit and Vegetable Garden Use, 1977	119
A-3	Summary of Human Inhalation Rates for Men, Women, and Children by Activity Level (m^3/hour)	123
A-4	Permeability Constants for Various Compounds	124
A-5	Typical Daily Soil Ingestion Rates for Children by Age Group	129
B-1	Possible Data Requirements for Estimation of Contaminant Release and Transport and Exposed Populations	136
B-2	Index to Variable Terms	139

List of Figures

Number		Page
1-1	Overview of the Integrated Exposure Assessment Process	2
2-1	Contaminant Release Decision Network: Contaminants in Soil	9
2-2	Contaminant Release Decision Network: Contaminants Above-Ground	11
2-3	Mean Number of Days Per Year with ≥0.01 Inches of Precipitation (i.e., "wet days")	15
2-4	Slope Effect Chart Applicable to Areas A-1 in Washington, Oregon, and Idaho, and all of A-3	24
2-5	Soil Moisture-Soil Temperature Regimes of the Western United States	24
2-6	Slope Effect Chart for Areas Where Figure 2-5 is Not Applicable	24
3-1	Environmental Fate Screening Assessment Decision Network: Atmosphere	37
3-2	Environmental Fate Screening Assessment Decision Network: Surface Water	39
3-3	Environmental Fate Screening Assessment Decision Network: Soils and Ground-water	41
3-4	Environmental Fate Screening Assessment Decision Network: Food Chain	42
3-5	Horizontal Dispersion Coefficient as a Function of Downwind Distance from the Source	43
3-6	Vertical Dispersion Coefficient as a Function of Downwind Distance from the Source	44
3-7	Area Within Isopleths for a Ground-Level Source	47
3-8	Nomograph for Solutions of Time, Distance, and Concentration for Any Point Along the Principal Direction of Ground-water Flow	78
A-1	Exposed Populations Decision Network	115
A-2	Quantitative Exposed Population Analysis	117

Foreword

The Superfund Exposure Assessment Manual presents an integrated method to help Remedial Project Managers and their contractors define the three major components involved in assessing human population exposure to contaminants released from uncontrolled hazardous waste sites:

1. Analysis of toxic contaminant releases;
2. Determination of the environmental fate of such contaminants; and
3. Evaluation of the nature and magnitude of exposure to toxic contaminants.

This report provides guidance for the development of exposure assessments using monitoring data (which may provide the most dependable basis for evaluating some existing exposure levels), as well as modeling techniques to predict exposure over time.

Executive Summary

The analytical process outlined in the Superfund Exposure Assessment Manual provides a framework for the assessment of exposure to contaminants at or migrating from uncontrolled hazardous waste sites. The application of both monitoring and modeling procedures to the exposure assessment process is outlined. This process considers all contaminant releases and exposure routes and assures that an adequate level of analytical detail is applied to support the human health risk assessment process.

The analytical process is structured in five segments:

1. Analysis of contaminant releases from a subject site into environmental media;
2. Evaluation of the transport and environmental fate of the contaminants released;
3. Identification, enumeration, and characterization of potentially exposed populations;
4. Integrated exposure analysis; and
5. Uncertainty analysis.

The Superfund Exposure Assessment Manual supports the development of exposure assessments that are consistent from site to site, and provides a means of documenting that each site receives adequate evaluation. The procedures presented reflect current (at the time of publication) state-of-the-art methods for conducting an exposure assessment. However, it is important for the analyst to recognize that exposure assessment is a developing science. Although the overall protocol for conducting exposure assessments at Superfund sites will not change significantly over time and the basic parameters needed as input to the analysis are not likely to change, alternative analytical methods may be developed for many parts of the assessment. The methods presented in this manual can serve as a benchmark against which such new methods can be compared.

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Chapter 1
Introduction

1.1 Purpose

The Superfund Exposure Assessment Manual provides Remedial Project Managers (RPMs) with the guidance necessary to conduct exposure assessments that meet the needs of the Superfund human health risk evaluation process. Specifically, the manual:

1. Provides an overall description of the integrated exposure assessment process as it is applied to uncontrolled hazardous waste sites; and

2. Serves as a source of reference concerning the use of estimation procedures and computer modeling techniques for the analysis of uncontrolled sites.

This manual provides guidance for the assessment of human population health risk only. Guidance for ecological risk assessment will be provided separately.

1.2 Background

The Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA - 42 USC 9601 et. seq.), as amended by the Superfund Amendments and Reauthorization Act of 1986 (SARA), was enacted to provide the Federal Government with the authority to respond to releases or threatened releases of hazardous substances, pollutants, or contaminants into the environment. As prescribed in the revised National Contingency Plan (see 47 FR 137, July 16, 1982), all sites designated for in-depth evaluation are included on the National Priorities List. These sites are evaluated for remedial action through the application of a Remedial Investigation, which defines the nature and extent of contamination, and a Feasibility Study, in which potential remedial alternatives are developed and analyzed. Guidance for conducting these two major components of the remedial response process is provided in USEPA (1985a and 1985b, respectively - currently under revision). As discussed in that guidance, a part of the Feasibility Study is the development of a risk assessment that projects those health impacts resulting from the uncontrolled site. The risk assessment is based on the results of a site exposure assessment, which evaluates:

1. The type and extent of contaminant release from a site to environmental media;

2. The environmental transport and transformation of contaminants following release; and

3. Implications of the resulting contact with exposed populations.

Section 110 of SARA mandates that health assessments be conducted by the Agency for Toxic Substances and Disease Registry for all sites on the National Priorities List. These health assessments can be based on the results of site-specific exposure assessments. The exposure assessment, therefore, is an analytical tool that is used to comply with the mandates of CERCLA.

1.3 Scope

This manual provides guidance for the use (but not the acquisition) of field data in the exposure assessment process. It does not serve as an all-encompassing guide to the use of computer models in the site remediation process, or direct the analysis of health risks that result from predicted exposure. This manual is intended to be used in conjunction with other related guidance, such as that for the acquisition of field data.[1] As detailed in USEPA (1987a), field sampling Data Quality Objectives (DQOs) establish a phased sampling strategy designed to guide the efficient acquisition of field data for site-specific exposure and public health assessments, and provide sampling plan guidance addressing the location of sampling points. Field operating procedures for obtaining and handling samples have also been developed (USEPA 1987b). Other references, (USEPA 1986a, 1986b, 1987c, and 1987d), address the utility, applications, and limitations of computer models for predicting contaminant concentrations and transport through various environmental media. The process for

developing a human health risk assessment for Superfund sites has been detailed in USEPA (1985c).

When conducting a comprehensive risk assessment, the analyst will need to refer to all of the above-cited guidance. While none of these guidance manuals stands alone, taken as a whole, they provide an overall, integrated approach to analysis of site contamination and health risk.

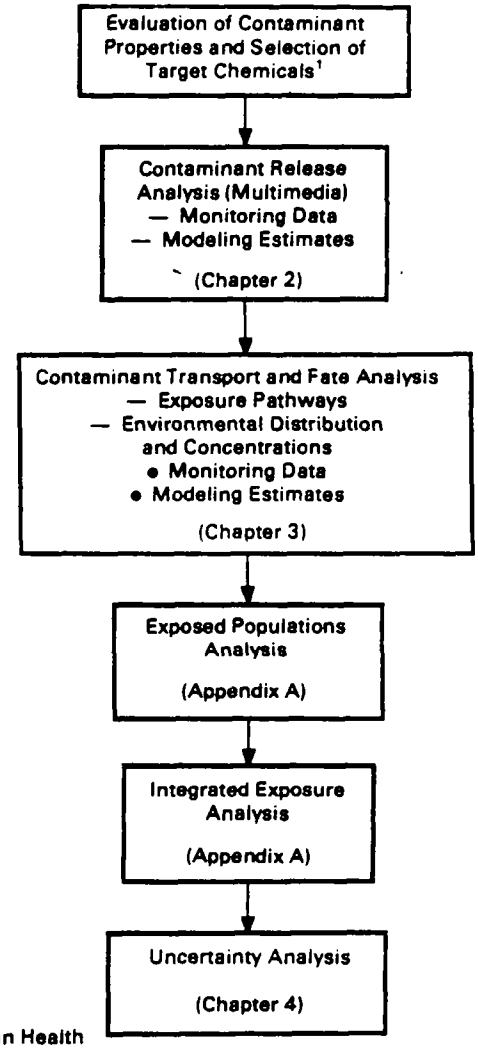
1.4 Use of the Manual

This manual is used to apply state-of-the-art exposure assessment procedures to the unique analytical needs of uncontrolled hazardous waste sites. The ultimate goal of human exposure assessment at Superfund sites is the determination of the type and magnitude of potential exposure to contaminants present at and migrating from the site. To achieve this goal, many sites may require a mix of qualitative and quantitative exposure analysis. The latter may range from simple analytical techniques (e.g., contaminant release or dispersion estimation equations) to more complicated computer modeling approaches.

The general procedure for conducting an integrated exposure analysis is illustrated in Figure 1-1. This procedure is based on EPA's published Guidelines for Exposure Assessment (USEPA 1986c) and other related guidance (USEPA 1985d-i) and is an adaptation of that process to the analytical problems posed by abandoned hazardous waste sites. As previously mentioned, target chemicals are selected as part of the human health risk assessment process (see USEPA 1985c). Once these chemicals are chosen, the exposure assessment proceeds through the following stages:

1. Contaminant Release Analysis
   Each on-site release point is identified for every target chemical, and the level of release (mass loading) to each environmental medium is determined. Determination of contaminant release may be made either by direct measurement (monitoring) of such releases or by estimation. Although difficult to achieve for all media, monitored release values provide a more sound basis for projection of contaminant migration later in the exposure assessment process than do modeled estimates. When it is not possible to obtain measured release rates, estimates can be based on measurements of contaminant concentrations in pertinent source media (e.g., estimates of contaminant release to ground water based on measured concentrations in contaminated soil). The results of the contaminant release analysis provide the basis for evaluating the potential for contaminant transport, transformation, and environmental fate.

Figure 1-1. Overview of the integrated exposure assessment process.



[1]Part of Human Health Risk Assessment Process. Refer to USEPA (1985c).

2. Contaminant Transport and Fate Analysis
   This analysis describes the extent and magnitude of environmental contamination (i.e., contaminant concentrations in specific environmental media). When possible, direct measurement of contaminant concentrations is preferred, and collection of samples during site evaluation will provide a clear basis for determining exposure potential for some exposure routes. However, the human health risk assessment process also requires projection of potential exposure over a lifetime (see Section 1-5), which can only be accomplished using estimation procedures.

3. Exposed Populations Analysis
The results of contaminant transport and fate analysis allow the analyst to evaluate populations contacting chemicals emanating from the site. Analysis of exposed populations involves the identification, enumeration, and characterization of those population segments likely to be exposed. The goal of this analysis is not only to delineate those populations coming into contact with contaminants emanating from the site, but also to determine how and with what frequency and duration such contact occurs.

4. Integrated Exposure Analysis
In this step, the individual chemical-specific exposure estimates for each exposure route (i.e., inhalation, ingestion, and dermal contact) are developed. For each exposed population, all exposures to each hazardous substance are identified. In cases in which a population group experiences more than one exposure by a given route, exposures are summed to develop a cumulative exposure value for the route involved. For example, persons who reside in the vicinity of a Superfund site may experience dermal exposure to a given contaminant directly on site as well as directly through basement seepage, and exposures via both of these routes should be summed for exposure integration purposes.

5. Uncertainty Analysis
The exposure assessment concludes with an analysis of uncertainty. In this analysis each step in the assessment is reviewed to identify any uncertainties involved and to evaluate their separate and cumulative impact on assessment results. Uncertainties may result from the use of default values for analytical input parameters, from the use of simplified estimation procedures as opposed to more rigorous computer analysis or monitoring-based analysis, from an inability to define exposed populations with confidence, etc. The uncertainty analysis provides necessary input for remedial decisionmakers who must evaluate the results of the exposure assessment with regard to their implications for potential risks associated with the uncontrolled site and appropriate remedial alternative selection

This manual is intended to be used in conjunction with various other guidance to conduct Superfund site Remedial Investigations and Feasibility Studies. The use of this manual is particularly linked to the Public Health Evaluation Manual. The two are intended to be used as two parts of the same process: the analysis of health impacts resulting from uncontrolled hazardous waste sites. In conducting a Superfund evaluation of exposure and public health impact, the analyst initially applies the indicator chemical selection process* outlined in the Superfund Public Health Evaluation Manual to select the chemicals on which the site analyses will focus. Once the chemicals have been selected, the analytical framework of the Superfund Exposure Assessment Manual is applied. Following completion of the exposure assessment, the analyst returns to the Superfund Public Health Evaluation Manual for guidance in determining the degree of human health risk for each exposed population.

The user of this manual should understand that these analytical procedures are intended to be applied site-specifically. No two sites will be exactly alike in terms of the extent and complexity of contamination, of contaminant migration, or of potentially exposed populations. Therefore, the specific analytical procedures to be applied in all Superfund exposure assessments cannot be fixed in general. Instead the approach and methods applied to conducting an exposure assessment must be tailored to address existing site conditions. In some situations contaminant releases or exposure routes may be adequately addressed by applying only screening procedures. In other cases more complex, quantitative evaluation will be necessary.

The Superfund Public Health Evaluation Manual (USEPA 1985c) lists five factors affecting the degree of analytical complexity for site analyses:

1. Number and identity of chemicals present;

2. Availability of appropriate standards and/or toxicity data;

3. Number and complexity of exposure pathways (including complexity of release sources and transport media);

4. Necessity for precision of the results; and

5. Quality and quantity of available monitoring data.

Simplified analyses may be used in the following instances: only a small number of chemicals must be evaluated; environmental standards or criteria for chemicals under study are available; a small number of exposure pathways are present; release and transport processes are relatively simple; or there is a limited need for detail and precision in the assessment results (e.g., screening studies). Conversely, sites that have many contaminants for which no environmental standards or criteria are available, that exhibit multiple exposure pathways, that have complex contaminant release and transport processes in effect, or that require analytical results in great detail and precision will require more

* Selection of indicator chemicals will be required only at those sites where the number of contaminants present is too large to individually evaluate exposure to each.

complex, quantitative analytical methods. Most sites will fall somewhere between these two extremes.

Procedures presented in this manual for conducting quantitative analyses include both simplified "desk top" approaches for developing order-of-magnitude estimates and more resource-intensive, in-depth approaches. Computer modeling and site monitoring are included. Generally, it is appropriate to apply simplified analysis to all pertinent exposure routes at the beginning of quantitative evaluations so that those causing greatest concern can be identified for subsequent in-depth analysis.

It is important to understand that analysis of exposure and resultant health impact is often a complex process in which selection and application of the most appropriate analytical tools, as well as the insightful interpretation of their results, can be critical. The U.S. EPA encourages ongoing communication between site analysts and experts in various exposure and health impact assessment fields. Thus, when questions arise regarding the utility of a particular model or mathematical solution, it is recommended that the analyst review the pertinent sections described in this manual or contact the Toxics Integration Branch of the Hazardous Site Evaluation Division of the Office of Emergency and Remedial Response (FTS 475-9486). In addition, Table 1-1 lists specific EPA contacts who can provide insight into particular site assessment problems.

In developing this manual, an attempt was made to compile analytical methods appropriate for assessing exposure to chemicals migrating from uncontrolled hazardous waste facilities. There are limitations to the application of these analytical tools and to the interpretation of the results obtained, including:

1. While some of these tools have been developed specifically for application to Superfund sites, others were originally developed for different purposes and had to be adapted or directly applied to evaluation of conditions present at uncontrolled hazardous waste sites. The analyst must be careful in interpreting the results obtained from application of these tools and must consider their inherent uncertainties.

2. This manual assumes that the analyst has a strong technical background in engineering or the sciences. This background is essential to ensure that analyses are carried out in a technically sound fashion and that interpretations of the results obtained are realistic.

3. It was not possible to include discussion of all technical limitations and caveats pertaining to each analytical tool or procedure reviewed in this manual. It may be beneficial for the analyst to obtain and review the original source documentation cited for analytical components.

4. Results obtained through application of these tools must be interpreted based on conditions at the site being analyzed. These tools are provided to aid the analyst in making decisions, not to make decisions for the analyst. When possible, models used in analyzing a given site should be verified with field monitoring data that test and validate model predictions at that site.

5. The approach to conducting exposure assessments outlined in this manual is conservative as are human health risk studies. However, the analyst needs to be sensitive to and to compensate, at least qualitatively, for the additive effect of multiple conservation assumptions. The degree of conservatism should not be so extreme that the conclusions drawn from the analysis are unrealistic.

1.5 Timeframe of Analysis

Quantitative exposure assessments generate estimates of the long-term (chronic daily intake) and short-term (subchronic daily intake) exposure to contaminants. The output of each analytical component (contaminant release, environmental fate, etc.) must be expressed in the same long-term and short-term form. Long-term releases are defined as the release rates of each contaminant migrating from the site averaged over an assumed 70-year human lifetime. Short-term contaminant releases are defined (USEPA 1985c) as those that occur over a short period (usually 10 to 90 days) during the first year following site investigation.

1.6 Analysis of Exposure Associated with Remedial Actions

The analytical tools presented in this Superfund Exposure Assessment Manual are those appropriate for analyzing exposure associated with the baseline condition (i.e., the uncontrolled site prior to implementation of any remedial action). It should be noted, however, that waste treatment processes used as part of a remediation strategy can themselves contribute significant releases of contaminants to the environment. Stripping volatiles from wastewaters, for example, generally involves artificial acceleration of the natural volatilization process, resulting in forced transfer of the volatile contaminants from wastewater to air. Thus, analysts must evaluate the engineering design of each remedial alternative to determine the level of contaminant release associated with its implementation. The user of this manual should refer to Farino et al. (1983) for a discussion of methods to estimate wastewater treatment air emissions. When incinerating toxic wastes other than those containing PCBs, Destruction and Removal Efficiency (DRE)

Table 1-1. Technical Resource Contacts for Superfund Exposure Assessments

Office	Commercial phone number	FTS phone number
I. U.S. Environmental Protection Agency:		
Office of Air Quality Planning and Standards; Research Triangle Park, N.C.	(919) 541-5381	629-5381
Office of Toxic Substances; Washington, D.C.	(202) 382-3886	382-3886
Office of Research and Development, Exposure Assessment Group; Washington, D.C.	(202) 475-8919	475-8919
Office of Research and Development, Hazardous Waste Engineering Research Laboratory; Cincinnati, Ohio	(513) 569-7418	684-7418
Environmental Research Laboratory; Ada, Okla.	(405) 332-8800	743-2011
Environmental Research Laboratory; Athens, Ga.	(404) 546-3134	250-3134
Center for Exposure Assessment Modeling; Athens, Ga.	(404) 546-3585	250-3546
II. Centers for Disease Control:		
Agency for Toxic Substances and Disease Registry; Atlanta, Ga.	(404) 454-4593	236-4593
III. International Ground Water Modeling Center:		
Holcomb Research Institute, Butler University; Indianapolis, Ind.	(317) 283-9458	-

requirements can be found in 40 CFR 264.343 (Environmental Protection Agency Regulations for Owners and Operators of Permitted Hazardous Waste Facilities; Subpart 0 - Incinerators). For incineration of wastes contaminated with PCBs, the analyst can refer to 40 CFR 761.70 (Polychlorinated Biphenyls (PCBs) Manufacturing, Processing, Distribution in Commerce, and Use Prohibitions - Incineration).

Well engineered remedial alternatives planned for uncontrolled hazardous waste sites are not expected in themselves to cause additional releases of toxic contaminants to ground-water systems. Even if an unexpected spill of toxics occurs when remedial action is taken, contaminant release should be slow enough to allow spilled substances to be isolated prior to their reaching the saturated zone. Short-term release of contaminants to air may occur while excavating contaminated soil and loading it for removal from the site. In such situations, the analyst should refer to USEPA (1983a), for release equations for material transfer.

The effectiveness of contaminant control, however, may vary among different remediation technologies. To evaluate post-remediation control effectiveness, many of the analytical procedures presented in this manual may be useful. For example, reductions in contaminant releases can be estimated by recalculating releases using altered (from the baseline case) site-specific input variables based on the remedial action under consideration. Alternatively, one can obtain a rougher approximation by applying the expected remedial action percent control (based on engineering experience) to the source release estimates calculated for the baseline case. In addition, the analyst should refer to USEPA (1985j) for a detailed discussion of both simplified analytical methods and numerical modeling approaches that can be used to estimate remedial effectiveness.

1.7 Organization of the Manual

The following chapters of this manual detail methods for evaluating exposure to chemicals migrating from Superfund sites. The body of the manual provides guidance for the qualitative and quantitative evaluation of contaminant release, migration, and fate in the environment, along with that for evaluating uncertainty in the analysis. Procedures for conducting exposed populations analysis and for developing an integrated exposure analysis are provided in appendices to this report.

Chapter 2
Contaminant Release Analysis

2.1 Introduction

This chapter provides guidance for the analysis of contaminant releases from uncontrolled hazardous waste sites. The goal of this analysis is to determine contaminant release rates to specific environmental media over time. The following sections address the release of contaminants to air, surface water, and ground water from wastes placed both above-ground and below-ground. In particular, guidance is provided for the evaluation of the following categories of contaminant releases:

1. Air releases:
   a. Fugitive dust resulting from:
      - Wind erosion of contaminated soils
      - Vehicular travel over contaminated unpaved roadways
   b. Volatilization releases from:
      - Covered landfills (with and without internal gas generation)
      - Spills, leaks, and landfarming
      - Lagoons
2. Surface water releases: contaminated runoff
3. Ground-water releases:
   a. Landfilled solids (lined or unlined)
   b. Landfilled liquids (lined or unlined)
   c. Lagoons (lined or unlined).

Contaminant release analysis is conducted in two stages - screening of contaminant release mechanisms and quantitative analysis. The screening, which is a qualitative evaluation of site conditions, identifies each potential contaminant release source, determines the environmental media affected by each release, and broadly defines the possible extent of the release. The following section is designed to establish a consistent basis for the qualitative screening of contaminant release from site to site.

Once the potential sources of on-site contaminant release have been screened, those requiring further evaluation are quantitatively analyzed. This may involve the application of a simplified "desk-top" estimation approach, or a more in-depth method such as computerized modeling or additional site monitoring. The goal of this analysis is to generate release rate estimates (mass per unit time) for each source of contaminant release. Release rate values are necessary as input for subsequent environmental fate analysis (see Chapter 3). Individual on-site releases of each contaminant are summed to generate an overall, medium-specific release rate for each chemical migrating from the site. Short-term (worst-case) release rates are developed, as are long-term rates (averaged over 70 years).

The simplified estimation procedures that follow allow the analyst to make release approximations based on chemical- and site-specific factors. However, these calculations do not take into account the full range of variables that affect on-site contaminant release. These approaches (with one exception) assume steady state conditions. They do not directly address the reduction in contaminants present (due to release losses), or the associated reduction in release loading over time corresponding with the decreasing contaminant reservoir.*

When possible, monitoring should be used to quantify rates of contaminant release. In some cases, however, this may not be feasible because methods to directly measure releases from certain settings are still being developed. Moreover, it may not always be possible to monitor contaminant releases under the conditions of concern (e.g., dust releases under high wind conditions, surface water runoff releases during storm events, etc.). It may often be necessary to estimate release rates in the exposure assessment process. All of the release rate estimation procedures presented here, however, require some monitored values as input. (Examples are measured contaminant concentrations in soil, soil characteristics.) The analyst should be aware of the need to develop a monitored data base that is adequate to support the needs of the contaminant release analysis portion of the exposure assessment.

In general, the procedures to estimate the rate of contaminant release are complete. When analyzing

* Estimation of the variation in the level of release over time is calculated separately. See Long-Term and Short-Term Release calculation subsections in this chapter.

wind erosion releases, however, the analyst should consult other published guidance that addresses the application of the wind erosion equation in various regions of the country. Depending on the location of a particular site, one of the following three manuals will be necessary:

- Craig and Turelle (1964): Great Plains
- Haynes (1966): Northeast
- Skidmore and Woodruff (1968): entire United States.

2.2 Contaminant Release Screening

The manner of waste placement at an abandoned site determines whether contaminant release* occurs by any or all of the mechanisms summarized in Table 2-1. In contaminant release screening, the likelihood of release from each source, the nature of the contaminants involved, and the probable magnitude of their release (relative to other on-site sources) are considered.

Figures 2-1 and 2-2 present the decision networks that guide contaminant release screening analysis. Figure 2-1 deals with contaminants in or under the soil and Figure 2-2 addresses above-ground wastes. Any release mechanisms evident at the site will require a further screening evaluation to determine the likely environmental fate of the contaminants involved (see Chapter 3).

2.2.1 Contaminants in Soil (see Figure 2-1)

The following numbered paragraphs help to interpret and apply the steps of the contaminant release decision network presented in Figure 2-1. Each paragraph refers to a particular numbered box in the figure.

1. Most uncontrolled hazardous waste sites will exhibit some degree of surface or subsurface soil contamination. This contamination may be the result of intentional waste disposal underground (landfilling) or in surface soils (surface application or landfarming), or it may be caused by unintentional waste releases from spills or leaks.

2. Landfilled wastes may become mobile if they are not contained in impervious containers, or if the containers are leaking. Release of such wastes may contaminate subsoils, ground water (through percolation), or air (through volatilization).

3. Landfilled wastes will be covered with soil; however, soil cover will not necessarily isolate wastes from the environment. If the cover can be penetrated by rainwater or run-on, wastes can be leached from the landfill cells and contaminate subsoils, ultimately reaching ground water. Similarly, the soil cover may not be deep enough to prevent the migration of volatile contaminants into the atmosphere. Estimations are that 60 percent of hazardous waste is in liquid (sludge) form (USEPA 1980a). Infiltrating rainwater can increase the migration rate of liquid or semiliquid materials by increasing the hydraulic head affecting them, as well as by the leaching of toxic components. Such factors as erosion or extreme drying (and cracking) can reduce the ability of a soil or clay cover to maintain the isolation of wastes. Also, contaminated soil may cover the waste cells themselves. When evaluating the potential for landfill releases, current conditions, along with the long-term integrity of the landfill and its soil cover, should be evaluated. If the landfill soil cover does not assure long-term

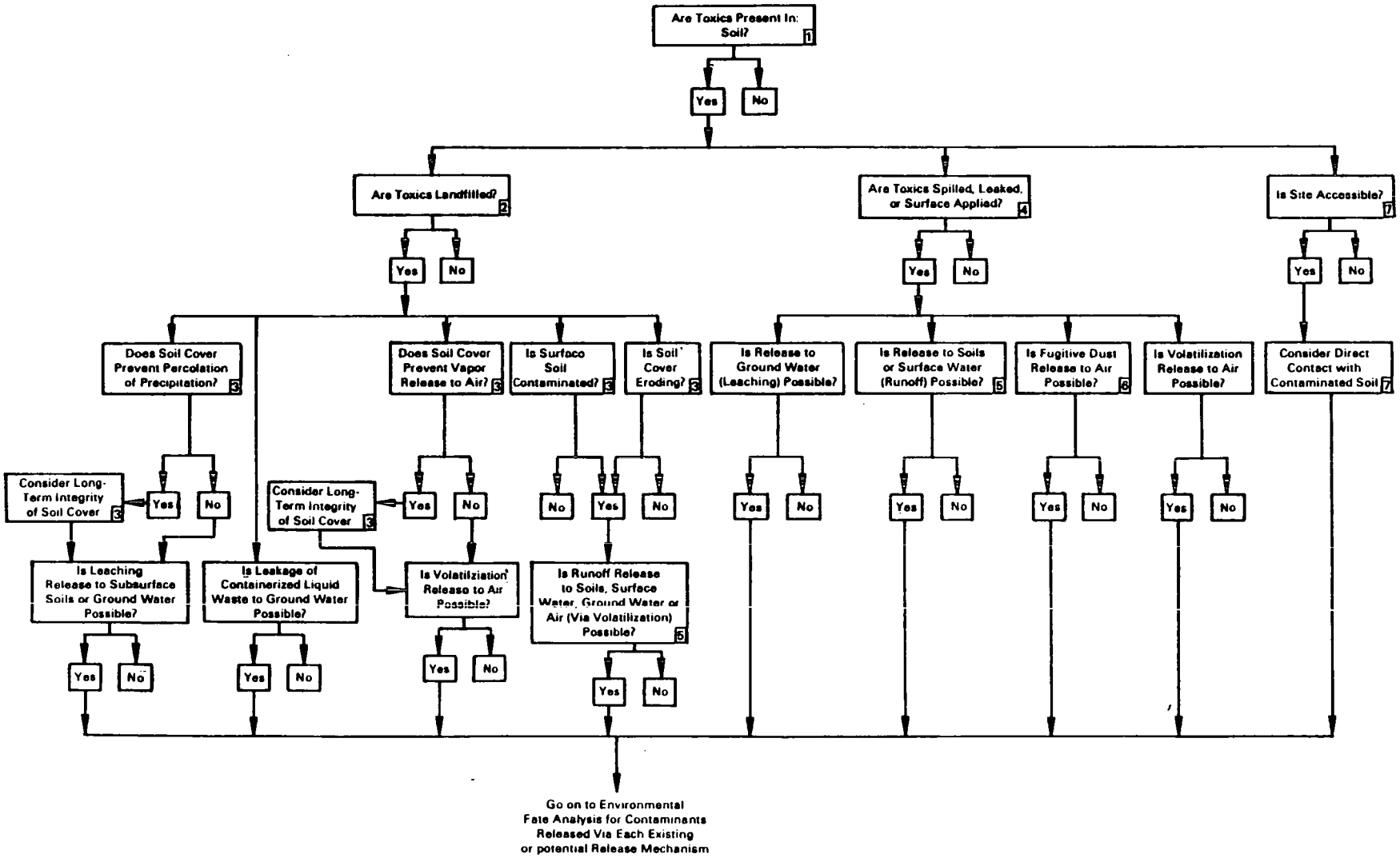
* For the purposes of this manual, contaminant "release" is defined as any process that results in migration of contaminants across the site boundary. Within this context, volatilization, generation of surface runoff, or leachate, are considered to be release mechanisms. Contaminant transport equates with those processes that carry released contaminants to points distant from the site.

Table 2-1. Potential Contaminant Release[1] Mechanisms

Process	Media directly affected (media indirectly affected)	Timeframe
Volatilization	Air	Chronic
Overland flow[2]	Soils, surface water (ground water)	Chronic, episodic
Direct discharge[3]	Soils, surface water (ground water)	Chronic, episodic
Leachate generation[4]	Soils, ground water	Chronic
Fugitive dust generation[5]	Air	Chronic, episodic
Generation of surface runoff	Soils, surface water (ground water)	Chronic, episodic
Combustion[3]	Air	Episodic

[1]See Section 2.2 for a definition of contaminant "release" as used in this manual.
[2]Impoundment overflow/failure, drum leakage, etc.
[3]Includes on-site treatment releases (e.g., wastewater/runoff treatment, incineration).
[4]Buried wastes, wastes stored above ground (leaks), land application, lagoons.
[5]Contaminated soils, particulate wastes.

Figure 2-1. **Contaminant release decision network: contaminants in soil.**



isolation of the wastes, one should evaluate the leachability and volatilization potential of the landfilled wastes.

4. At some hazardous wastes sites, toxic materials may have been purposefully incorporated into surface soils to promote their microbial destruction. In such cases, toxic components may still remain in the soil. At most sites, however, surface soils have become contaminated because of hazardous material spills or leaks during manufacturing, processing, storage, or transfer operations. In these situations, the potential for release of contaminants in surface soils through four mechanisms should be evaluated. These mechanisms are: (1) release of volatile components to the atmosphere (via evaporation); (2) release of toxic particulate matter (via wind erosion); (3) surface runoff-related releases; and (4) percolation of contaminants or leachate to ground water.

5. The percolation of contaminated runoff may contaminate surface soils and underlying ground water. Surface water systems may be similarly degraded by contaminated runoff inflow. Runoff may also serve as a source of volatilization release to air, although releases from contaminated soils would be expected to constitute a greater threat than that from contaminated runoff. Hydrophobic wastes may contaminate surface waterbodies by adsorbing onto soil material that can be eroded from the site and enter a waterbody in surface runoff. In a waterbody, sediment transport is much slower than is water movement, and contaminated sediments may remain in the vicinity of the contamination source for a long time.

6. Under high wind conditions, wind erosion may carry solid particulate wastes or soil particles with sorbed hydrophobic toxic materials from the site.

7. If the site is accessible, direct contact with contaminants may occur. Also children may ingest some contaminated soil during play. Such ingestion may result from "pica" behavior (i.e., intentional eating of soil by very young children) or from normal hand to mouth contact.

2.2.2 Contaminants Above-Ground

The following numbered paragraphs help to interpret and apply the steps of the contaminant release decision network presented in Figure 2-2. Each paragraph refers to a particular numbered box in the figure.

1. Wastes can be stored above-ground in lagoons/ponds, in containers (drums, tanks), or in piles. Unless containers effectively isolate wastes from the environment, above-ground storage can result in the direct introduction of contaminants into air, soils, surface water, or ground water.

2. Lagoons may introduce hazardous materials to the environment through a number of pathways. Erosion or overflow resulting from heavy rainfall can breach the lagoon and result in the outflow of liquid wastes that contaminate surface soils, ground water, and surface waterbodies. In addition, unlined lagoons may introduce toxics directly into ground water via percolation through the lagoon bottom. Also, because lagoons are uncovered, the release of volatile compounds to the atmosphere is a common problem.

3. Wastes stored above-ground in containers may not be effectively isolated from the environment. Over time, container corrosion and leakage occur. Leaked wastes will contaminate soils in the storage area; may percolate to ground water; or may contaminate surface runoff, which, in turn, can extend the area of soil contamination or can enter local surface waterbodies. Leaked materials may also evaporate into the atmosphere.

4. If the site is accessible to the public, direct contact with contaminants may occur. Also, children may ingest contaminated soils, either inadvertently or as a result of pica behavior.

2.3 Quantitative Analysis of Atmospheric Contamination

2.3.1 Fugitive Dust Emission Analysis

Emissions of contaminated fugitive dusts (airborne wastes or contaminated soil particles) originating at uncontrolled hazardous waste sites can result from a combination of such factors as (1) wind erosion of wastes and contaminated soils, and (2) vehicles traveling over contaminated, unpaved roads.

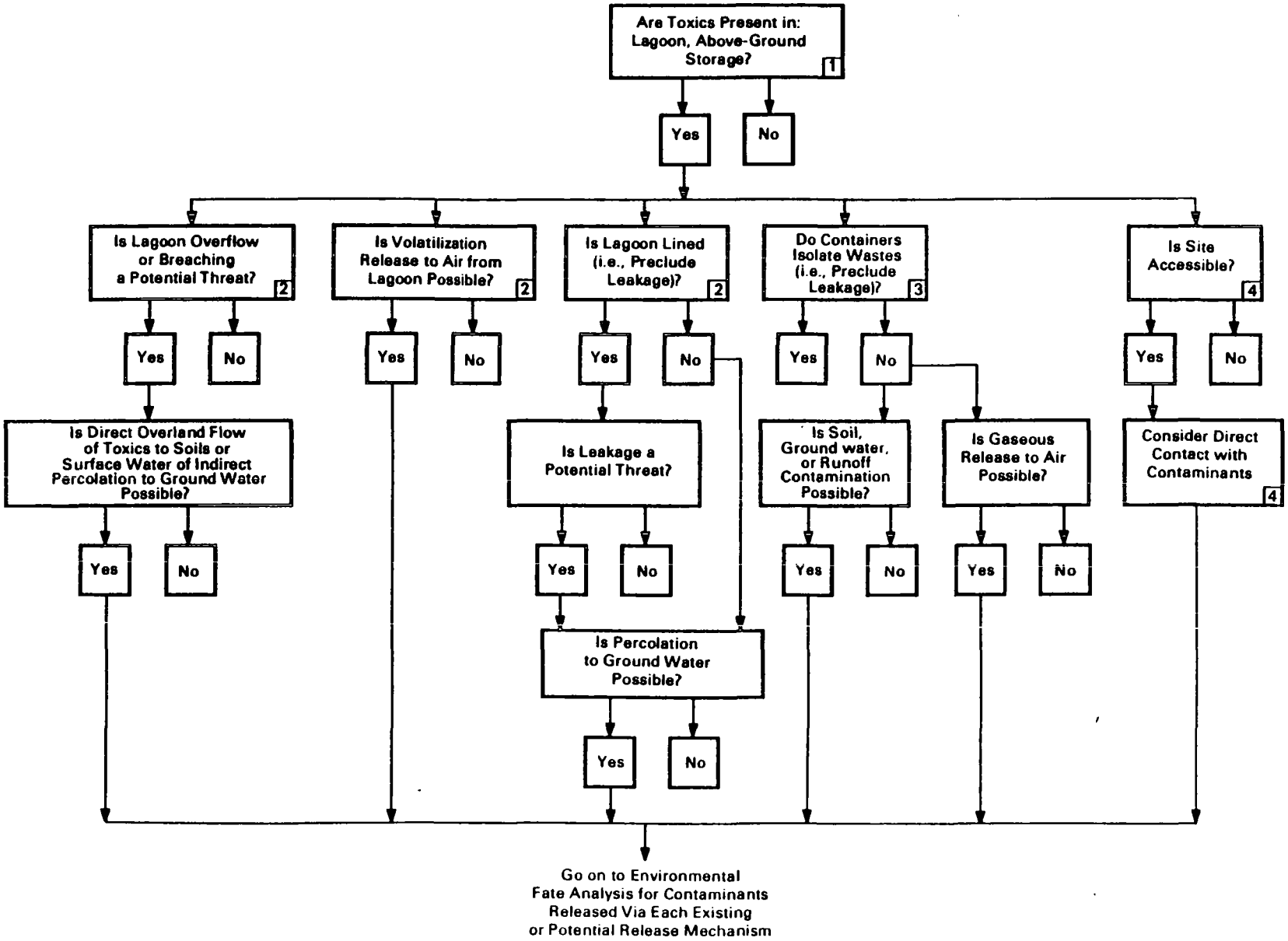
Methods for analyzing such contaminant releases are presented below.

2.3.1.1 Beginning Quantitative Analysis

The following procedures are useful in estimating total fugitive dust releases likely to result from the two factors cited above. Once total suspendible dust generation levels have been calculated using these equations, one can project the amounts of hazardous substances expected to enter the atmosphere in fugitive dust using either of the following approaches:

- Multiply the amount of dust generated by the weight percent of the toxic substance in soil or waste. This approach does not take into account factors relating to such aspects as particle size or adsorption potential, which can affect the amount

Figure 2-2. Contaminant release decision network: contaminants above-ground.



of contaminant actually entering the atmosphere as dust.

- Multiply the estimates for total dust generation by percentages (by weight) of the substances of concern in actual fugitive dust samples obtained with on-site air monitoring. This approach takes into account those chemical-specific and site-specific factors that affect release of contaminated dust in the field.

*(1) Wind Erosion Analysis**

Wind erosion of agricultural soils and, by extrapolation, other disturbed soils, depends upon a variety of factors. These include surface roughness and cloddiness; surface soil moisture content, kind, amount (and orientation, if applicable) of vegetative cover; wind velocity; and the amount of soil surface (length) exposed to the eroding wind force. The U.S. Soil Conservation Service (SCS) has developed a method to estimate wind erosion based on a series of graphs relating variables presented below. The graphical method for calculating wind erosion based on the functional relationship of these variables is not presented in this manual; instead, the analyst is directed to the Skidmore and Woodruff (1968) source document.

$$E = f(I', C', K', L', V) \qquad (2\text{-}1)$$

where

E = potential annual average wind erosion soil loss, (mass/area/time).
I' = soil erodibility index, (dimensionless).
C' = climatic factor, (dimensionless).
K' = soil ridge roughness factor, (dimensionless).
L' = field length along the prevailing wind direction, (feet).
V = vegetative cover factor, (dimensionless).

Multiplying E times the contaminated area will yield a release rate in units of mass per time.

Table 2-2 identifies the factors that determine the values of the five variables used in the SCS equation. Note that the vegetative cover factor (V) specifically applies to crop residues, and care must be taken when extrapolating to the cover conditions present at uncontrolled waste sites. For Remedial Investigation and Feasibility Study estimation purposes, one can use a "zero pounds per acre" vegetative cover value. This assumes a worst-case situation (from a vegetation-related wind attenuation perspective) and provides a conservative estimate of contaminated fugitive dust release.

A series of publications issued by the U.S. Department of Agriculture provides directions for applying this equation to a site-specific situation. Craig and Turelle (1964) present estimation procedures for the Great Plains; Haynes (1966) addresses the Northeast; and Skidmore and Woodruff (1968) offer procedures for the entire nation.

Although it is strongly recommended that site-specific soils data be obtained for each site under evaluation, it is not necessary to do so in order to obtain parameter values for use with the wind erosion equation (or other fugitive dust generation equations). Instead, when necessary, soils data can be obtained from the local Soil Conservation Service office. SCS has on record a range of pertinent soils data for sites across the country where soil surveys have been conducted. In addition, SCS maintains an extensive computerized soil properties data base called the Soils 5 File. This data base lists estimated soils data, based on surveys of surrounding soils properties, for areas where surveys have not been conducted to date. These data are readily available from local SCS officials. Users of this manual should consult SCS to obtain more detailed information regarding the nature and accessibility of information contained in the soil surveys and the Soils 5 File.

The SCS wind erosion equation is one of a number of approaches for estimating particulate release from abandoned hazardous materials facilities. One such source (Cowherd et al. 1985) is specifically designed to guide rapid (less than 24 hours) evaluation of the potential degree of particulate emission from uncontrolled hazardous waste sites. This method uses an emission factor approach to estimate release and procedures adapted from computerized dispersion models for approximating concentration isopleths. Concentration estimates and Bureau of the Census data are used to identify the exposed population and estimate the level of exposure. This approach includes the three key components of exposure analysis: release rate estimation, contaminant migration analysis, and population exposure determination. However, Cowherd et al. (1985) caution that their method is designed for emergency evaluations or as a preliminary assessment tool, which may then be used in undertaking a more detailed investigation. Nevertheless, the degree of accuracy attained using this method is consistent with simplified quantitative estimation procedures. This approach provides the analyst with estimates of short-term (worst-case, 24-hour) release and exposure estimates, as well as long-term (average annual) estimates.*

The SCS wind erosion equation is designed to provide annual erosion losses only, and cannot be

* Applied to nonadhering, noncompacted contaminated soil or waste materials.

Table 2-2. Environmental Variables and Model Parameters for the Wind Erosion Equation

Equivalent SCS wind erosion equation primary wind erosion variables	Parameters
Soil erodibility index, I (function of soil particle size distribution; read from a table) Knoll erodibility, I_s (function of knoll slope steepness; read from a graph)	Soil and knoll erodibility, I' (equal to I x I_s)
Surface crust stability, F_s	Disregarded--crust is transient
Soil ridge roughness, K_r, (function of height, width, and spacing of clods and furrows)	Soil ridge roughness factor, K' (estimated by comparison to a set of standard photographs included in SCS wind erosion equation users' manuals)
Annual average wind velocity, v (read from map) Surface soil moisture, M (estimated using Thornthwaite's (1931) precipitation-evaporation index)	Local wind erosion climatic factor, C' (may be calculated but commonly read from maps of C')
Distance across field, D_f (field width in direction of primary erosive wind) Sheltered distance, D_b (calculated from barrier height upwind of field)	Field length, L' (the difference between D_f and D_b)
Quantity of vegetative cover, R' (mass of standing or fallen vegetative residue per unit area) Kind of vegetative cover, S (factor related to erosion-reducing effectiveness of residues from different crops) Orientation of vegetative cover, K_0 (factor relating erosion reduction to standing vs. fallen crop residues)	Equivalent vegetative cover, V (the product of R', S, and K_0) - can often be assumed = 0 for abandoned waste sites (see text)

Source: Smith et al. 1982.

reliably altered to generate short-term estimates.* In addition, it cannot be used with data delineating climatic extremes for a given location, but must be based on average annual climatic data. Instead, for exposure assessment purposes the short-term release, estimated using the wind erosion equation, is assumed to equal the average release over the first year following site investigation.

The user of this manual should review Cowherd et al. (1985) and compare that method with the SCS wind erosion procedure before selecting an analytical approach for estimation of particulate contaminant release and related exposure. The analyst can also refer to USEPA (1983b), Farino et al. (1983), Sehmel (1980), and Smith et al. (1982) for a review of other possible approaches.

As noted in USEPA (1983b), the SCS wind equation computes the total wind erosion soil loss resulting from the combination of surface creep, saltation, and suspension. Although appropriate for studies of agricultural soil loss, in exposure evaluations the analyst is generally concerned only with that fraction of the total soil loss that consists of particles of suspendible, wind transportable, and inhalable size. When the wind erosion equation is used to estimate contaminated fugitive dust exposure situations, the total soil loss results obtained from the wind erosion equation must be adjusted (reduced) to reflect only that portion of the total soil loss that is suspendible and transportable over significant distances by wind.

Considerable discussion of the cut-off point for suspendible soil particle size exists in the literature (Sehmel 1980, Smith et al. 1982, and USEPA 1983a, b). As a group, particles ≤ 100 µm aerodynamic equivalent diameter include those that can be suspended by and transported in the wind and those that can be inhaled (see Miller et al. 1979 and USEPA 1986d for a discussion of the extent to which various particle sizes penetrate the human respiratory system). Particles in the 30 to 100 µm diameter range will often settle within a few hundred feet of the source (USEPA 1983a), while those particles ≤30 µm in diameter can be transported considerable distances downwind. To estimate inhalation exposure, only the inhalable fraction of suspended particulates (≤10 µm in diameter) must be considered.

For particles in the 2- to 20-µm size range, the particle size distribution of the parent soil determines the size distribution of suspended particles (Smith et al. 1982). Therefore, that proportion which is ≤10 µm in diameter can be determined based on the soil size distribution of the parent soil. It can be assumed that this proportion of the total soil loss, as calculated via the SCS wind erosion equation, is lost to suspension and is available for inhalation.

(2) Unpaved Roads Analysis

The following equation (USEPA 1983a) can be used to estimate fugitive dust releases associated with vehicles traveling on contaminated unpaved roads.

* Note: EPA (1985c) defines short-term concentrations to equate with a 10- to 90-day period. Thus, the 24-hour maximum exposure may not adequately represent subchronic exposures.

** Personal communication between Lee Schultz (Versar Inc.) and Thomas George (U.S. Soil Conservation Service), July 24, 1985.

$$E_{VT} = k(5.9)\left(\frac{s}{12}\right)\left(\frac{Sp}{30}\right)\left(\frac{W}{3}\right)^{0.7}\left(\frac{w}{4}\right)^{0.5}\left(\frac{365-Dp}{365}\right)$$

or in metric form (2-2)

$$E_{VT} = k(1.7)\left(\frac{s}{12}\right)\left(\frac{Sp}{48}\right)\left(\frac{W}{2.7}\right)^{0.7}\left(\frac{w}{4}\right)^{0.5}\left(\frac{365-Dp}{365}\right)$$

where

E_{VT} = emission factor for vehicular traffic, (lb/vehicle mile traveled; kg/vehicle kilometer traveled)
k = 0.45 = particle size multiplier for particles ≤ 10 µm (i.e., particles that may remain suspended once they become airborne and which can be inhaled into the respiratory system).*
s = silt content (of road surface material), (percent).**
Sp = mean vehicle speed, (mph; kph).
W = mean vehicle weight, (tons; Mg).
w = mean number of wheels.
Dp = number of days with at least 0.254 mm (0.01 in) of precipitation per year (see Figure 2-3).

The emission factor (E_{VT}) can be multiplied by a "vehicle kilometers traveled per time" value to generate a "dust release per time value." Short-term (maximum release) estimates can be made by using a reduced value of "Dp" in the equation to reflect assumed drought conditions at the site. Figure 2-3 reflects the range of average "Dp" values for locations in the U.S. Consultation with the local National Weather Service office may provide locale-specific insight into what "Dp" values should be used to represent dry years at the site. Long-term (average) releases can be estimated by using the annual average value for "Dp." USEPA (1983a) states that this equation is valid for situations that comply with the following source conditions:

- Road surface silt content = 4.3 - 20 percent;
- Mean vehicle weight = 3-157 tons (2.7-142 Mg);
- Mean vehicle speed = 13-40 mph (21-64 kph); and
- Mean number of wheels = 4-13.

For an overview of the utility and limitations associated with the application of emission factors to particulate release estimation problems, the user of this manual can refer to USEPA (1983a, b), Farino et al. (1983), Sehmel (1980), and Smith et al. (1982).

2.3.1.2 In-Depth Analysis
For contaminated fugitive dust emissions, in-depth analysis will consist of monitoring and modeling activities. Generally, air sampling will be conducted downwind and upwind of the uncontrolled hazardous waste site. The difference in particulate loading obtained at the two (or more) sampling locations will quantify the particulate mass loading attributable to the site alone (assuming that air sampling stations can be sited to eliminate interference from other sources). Using these data, either simple dispersion equations or computerized air dispersion modeling* can be used to back-calculate the emission level at a "virtual point source." The use of dispersion modeling to back calculate emission levels, however, is often quite unreliable because of the difficulty in obtaining accurate ambient monitoring and meteorological input data.

The virtual point source is a hypothetical source located upwind of the subject site that has a hypothetical release rate which would result in the contaminant concentrations observed at the uncontrolled hazardous waste site (area source). The virtual point source release rate can then be used in subsequent contaminant transport analysis for the subject site. The user of this manual should refer to USEPA (1983c) and Seely et al. (1983) for a detailed presentation of ambient air sampling strategies and procedures appropriate for abandoned hazardous waste facilities.

2.3.2 Volatilization Emission Analysis
Volatilization of contaminants at uncontrolled hazardous waste sites can occur at the following sources:

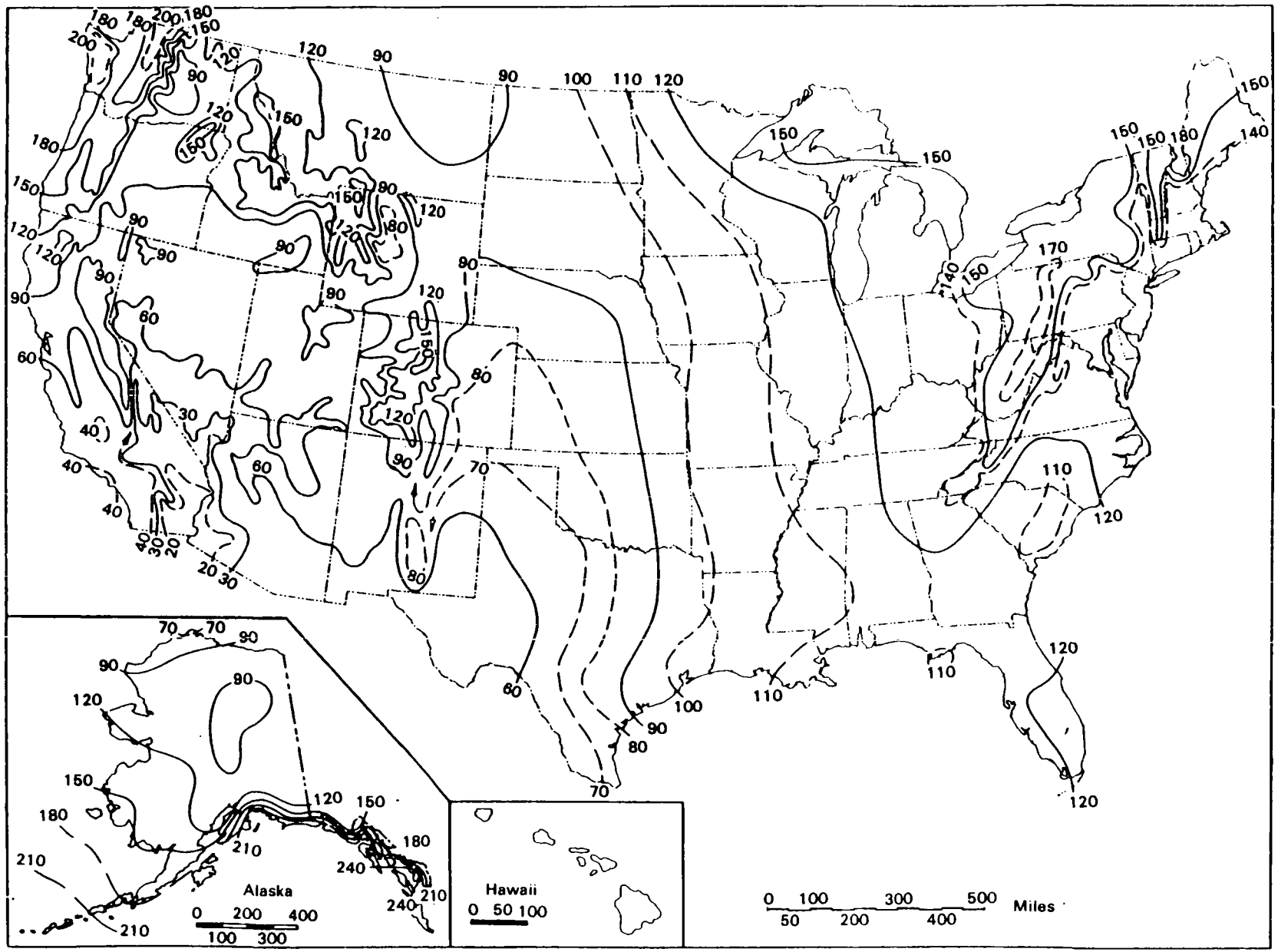
(1) Covered landfills - without internal gas generation;
(2) Covered landfills - with internal gas generation;
(3) Spills, leaks, landfarms - concentrated wastes on the surface or adhered to soil particles below the surface; and
(4) Lagoons - wastes dissolved in or mixed with water.

In the baseline situation, one or more of these sources will contribute to the overall air loading originating at the site, and will need to be controlled through remedial action.

2.3.2.1 Beginning Quantitative Analysis
This section presents simplified analytical procedures for estimating releases from the above source categories. Because the chemical properties of a given substance largely determine the volatilization rate, the equations presented require input of

* See EPA (1983a) for "k" values used when release of specific particle size groups other than ≤ 10 µm is desired.
** Soil silt content can be estimated from SCS Soils 5 File data by subtracting the "percent clay" value from the "percent material passing No. 200 sieve" value. (Personal communication between Lee Schultz (Versar Inc.), and Keith Young (U.S. Department of Agriculture, Soil Conservation Service), Washington, D.C., May 1, 1984.)

Figure 2-3. Mean number of days per year with ≥0.01 inches of precipitation (i.e., "wet days") (USDC 1968).



quantified property values. These data are available for many chemicals that may be present at uncontrolled hazardous waste sites, and are found in various chemical reference texts. In cases where chemical data are missing, the analyst must estimate the property values. This section provides equations for estimating certain requisite chemical properties. Comprehensive guidance for chemical property estimation is provided in reference materials such as Lyman et al. (1982). Readily accessible computerized systems are available to predict a range of pertinent chemical properties. The computerized Graphic Exposure Modeling System (GEMS), and its subsystem CHEMEST, is an example. The EPA Office of Toxic Substances in Washington, D.C. has developed and is managing this system. Essentially a computerized version of Lyman et al. (1982), it can be rapidly accessed to estimate the chemical characteristics necessary for volatilization estimation.

The user of this manual can refer to Farino et al. (1983) for a detailed review and evaluation of existing equations for estimating volatilization from uncontrolled hazardous waste sites. This report presents a survey of available air release models for volatile substances and a critical analysis of the applications and limitations of each.

(1) Landfills Without Internal Gas Generation

Equation 2-3 can be used to estimate volatile releases from covered landfills containing toxic materials alone, or toxic materials segregated from other landfilled nonhazardous wastes. Equations 2-4 through 2-7 are used to calculate certain input variables that are required to apply Equation 2-3. Farmer et al. (1978) developed an equation to estimate the effectiveness of various landfill cover types and depths in controlling volatile releases. This equation, based on Fick's First Law of steady state diffusion, assumes that diffusion into the atmosphere occurs at a plane surface where concentrations remain constant. It ignores biodegradation, transport in water, adsorption, and production of landfill gas. Diffusion of the toxic vapor through the soil cover is the controlling factor. It also assumes that there is a sufficient mass of toxicant in the landfill so that depletion of the contaminant will not reduce the emission rate.

Equation 2-3, simplified by Farmer et al. (USEPA 1980b), incorporates a number of assumptions (see Farino et al. 1983 for a complete discussion), such as completely dry soil (worst case) and zero concentration of volatilizing material at the soil surface. Shen (1981) converted Farmer's simplified equation for calculating the vapor flux rate to a form that provides a toxic vapor emission rate by multiplying the basic equation by the exposed contaminated surface area. In addition, Shen modified the equation to allow calculation of the volatilization rate of a specific component of the overall toxic mixture by multiplying by the weight fraction of the component in the mixture. However, as pointed out by Farino et al. (1983), a more accurate approach would be to multiply by the mole fraction of the toxic component in the buried mixture. Thus, Farmer's equation, as modified by Shen (1981) and Farino et al. (1983), is:

$$E_i = D_i C_{si} A \left(P_t^{4/3} \right) \frac{M_i}{d_{sc}} \qquad (2\text{-}3)$$

where

E_i = emission rate of component i, (g/sec).
D_i = diffusion coefficient of component i in air, (cm^2/sec).
C_{si} = saturation vapor concentration of component i, (g/cm^3).
A = exposed area, (cm^2).
P_t = total soil porosity, (dimensionless).
M_i = mole fraction of toxic component i in the waste,(gmole/gmole).
d_{sc} = effective depth of soil cover, (cm).

Note that total soil porosity, rather than air-filled soil porosity, is used in this equation. The presence of water in a soil cover will tend to decrease the flux rate of a volatile compound by effectively decreasing the porosity, and also by increasing the geometric complexity of the soil pore system (because water adheres to soil particles), thus effectively increasing the vapor path (USEPA 1980b). Farmer et al. suggest, however, that when using their equation to design a landfill cover, the total porosity value be used (USEPA 1980b), thereby designing for the worst case (i.e., dry conditions). In most instances, it will be appropriate to apply this same worst-case logic to the analysis of volatilization release from landfilled wastes, assume that landfill cover soils are dry, and use a value for total porosity in Equation 2-3. It is recognized, however, that there may be situations where it can be shown that cover soils exist in a wet condition more often than in a dry one. In these cases, the air-filled soil porosity (Pa) may be more appropriate, and this value can be substituted for P_t in Equation 2-3 when analyzing volatilization release.

If not provided in existing literature, D_i, a compound's diffusion coefficient (required for the above equation), can be calculated by Fuller's Method (Perry and Chilton 1973):

* Although computerized dispersion modeling can be used to obtain contaminant release rates, it is primarily a tool for determining contaminant atmospheric fate. Thus, refer to Chapter 3, Environmental Fate Analysis, for detailed discussions of air dispersion models applicable to uncontrolled hazardous waste facilities.

$$D_i = \frac{0.001T^{1.75}\sqrt{\frac{1}{MW_i} + \frac{1}{MW_a}}}{P_a[(\Sigma V_1)^{1/3} + (\Sigma V_a)^{1/3}]^2} \qquad (2\text{-}4)$$

where

T	=	absolute temperature, (°K).
$MW_i; MW_a$	=	molecular weights of toxic substance and air (28.8), respectively, (g/mole).
P_a	=	absolute pressure, (atm).
$\Sigma V_1; \Sigma V_a$	=	molecular diffusion volumes of toxic substance and air (20.1). This is the sum of the atomic diffusion volumes of the compound components, (cm^3/mole).

To estimate short-term (maximum) release rates, use a value for the temperature that reflects the expected summer maximum temperatures. Annual average temperatures should be used to initially estimate long-term (average) release rates. This initial estimated long-term release value will be revised as described in Section 2.3.3 to develop final long-term release estimates.

Relevant atomic diffusion volumes for use in estimating D_i are (Perry and Chilton 1973):

C = 16.5	Cl = 19.5	Aromatic ring	= -20.2
H = 1.98	Br = 35.0	Heterocyclic ring	= - 20.2
O = 5.48	F = 25.0*		
N = 5.69	S = 17.0		

Table 2-3 presents diffusion coefficients that have been calculated for a variety of compounds, some of which may be present at abandoned sites.

An alternative method (Shen 1981) for approximating D_i involves the identification of a compound listed in Table 2-3 that has a molecular weight and molecular diffusion volume (calculated) similar to those of the toxic substance under evaluation. The unknown diffusion coefficient can then be calculated using:

$$D_i = D'\left(\frac{MW'}{MW_i}\right)^{\frac{1}{2}} \qquad (2\text{-}5)$$

where

D_i	=	diffusion coefficient of the compound to be estimated from the known D'.
D'	=	diffusion coefficient of a compound that can be found in the table, the molecular weight and atomic diffusion, volume of which are close to that of the unknown.
MW'	=	molecular weight of the selected compound D'.
MW_i	=	molecular weight of the compound to be estimated.

Total soil porosity, P_t, can be calculated as follows (USEPA 1980b):

$$P_t = 1 - \frac{\beta}{\rho} \qquad (2\text{-}6)$$

where

P_t	=	total soil porosity, (dimensionless).
β	=	soil bulk density,* (g/cm^3): generally between 1.0 and 2.0 g/cm^3.
ρ	=	particle density, (g/cm^3): usually 2.65 g/cm^3 used for most mineral material.

For estimation, P_t can be assumed to be approximately 0.55 for dry, non-compacted soils, and about 0.35 for compacted soils. This same value (0.35) is also appropriate for use as a generic air-filled soil porosity (Pa) when analyzing the volatilization release from soils with a high moisture content (Shen 1981). Alternatively, the local Soil Conservation Service office can be contacted to obtain site-specific estimated air-filled soil porosity values for specific locations.

Saturation vapor concentration, C_{si}, can be determined by (USEPA 1980b):

$$C_{si} = \frac{pMW_i}{RT} \qquad (2\text{-}7)$$

where

C_{si}	=	saturation vapor concentration of component i, (g/cm^3).
p	=	vapor pressure of the chemical,** (mm Hg).
MW_i	=	mole weight of component i, (g/mole).
R	=	molar gas constant, (62,361 mm Hg-cm^3/mole-°K).
T	=	absolute temperature, (K).

Again, use maximum summer temperatures to estimate short-term release and annual average temperatures to initially estimate long-term release.

* This value is from Shen (1981).

* Values for soil bulk density for specified locations can be obtained from the U.S. Soil Conservation Service, Soils 5 File data base.

** If the vapor pressure of a chemical under consideration is not available in standard reference texts, estimate it as described in Lyman et al. (1982).

Table 2-3. Diffusion Coefficients of Selected Organic Compounds

Compound	Formula	Molecular weight	Atomic diffusion volume	Diffusion coefficients (cm^2/sec) at 10°C	at 30°C	at 50°C
Acetaldehyde	C_2H_4O	44	46.40	.11758	.13249	.14816
Acetic acid	$C_2H_4O_2$	60	51.88	.10655	.12007	.13427
Acetone	C_3H_6O	58	66.86	.09699	.10930	.12223
Aniline	C_6H_7N	93	118.55	.07157	.08065	.09019
Benzene	C_6H_6	78	90.68	.08195	.09234	.10327
Bromoethane	CH_3Br	95	57.44	.09611	.10830	.12111
Bromoform	$CHBr_3$	118	53.48	.09655	.10880	.12167
Carbon tetrachloride	CCl_4	154	94.50	.07500	.08451	.09451
Chlorobenzene	C_6H_5Cl	113	128.40	.06769	.07627	.08530
Chloroethane	C_2H_5Cl	65	62.40	.09789	.11031	.12336
Chloroform	$CHCl_3$	120	76.89	.08345	.09404	.10517
Chloromethane	CH_3Cl	51	57.94	.10496	.11827	.13226
Cyclohexane	C_6H_{12}	84	122.76	.07139	.08045	.08996
Dichloroethane	$C_2H_4Cl_2$	99	75.96	.08557	.09643	.10784
Dichloroethylene	$C_2H_2Cl_2$	97	106.96	.07442	.08386	09377
Dichloropropalene	$C_3H_6Cl_2$	113	100.38	.07519	.08473	.09475
Dimethylamine	C_2H_7N	45	52.55	.11161	.12577	.14065
Ethanol	C_2H_6O	46	50.36	.11297	.12730	.14236
Ethyl acetate	$C_4H_8O_2$	88	92.80	.07991	.09005	.10070
Ethylamine	C_2H_7N	45	52.55	.11161	.12577	.14065
Ethylbenzene	C_8H_{10}	116	151.80	.06274	.07070	.07906
Fluorotoluene	C_7H_7F	110	154.36	.06262	.07056	.07891
Heptane	C_7H_{16}	100	146.86	.06467	.07287	.08149
Hexane	C_6H_{14}	86	126.72	.07021	.07912	.08848
Isopropanol	C_3H_8O	60	37.82	.12004	.13526	.15126
Methanol	CH_4O	32	29.90	.14808	.16686	.18660
Methyl acetate	$C_3H_6O_2$	74	72.34	.09054	.10203	.11410
Methyl chloride	CH_2Cl_2	85	59.46	.09610	.10830	.12111
Methylethyl ketone	C_4H_8O	72	87.32	.08417	.09485	.10607
PCB (1 Cl)	$C_{12}H_9Cl$	189	235.32	.04944	.05571	.06230
Pentane	C_5H_{12}	72	106.26	.07753	.08737	.09770
Phenol	C_6H_6O	84	96.16	.07919	.08924	.09980
Styrene	C_8H_8	104	137.84	.06620	.07460	.08343
Tetrachloroethane	$C_2H_2Cl_4$	168	1143.96	.06858	.07729	.08643
Tetrachloroethylene	C_2Cl_4	166	111.00	.06968	.07852	.08781
Toluene	C_7H_8	92	111.14	.07367	.08301	.09283
Tricyhloroethane	$C_2H_3Cl_3$	133	97.44	.07496	.08447	.09446
Trichloroethylene	C_2HCl_3	131	93.48	.07638	.08606	.09625
Trichlorofluoromethane	CCl_3F	138	100.00	.07391	.08329	.09314
Vinyl chloride	C_2H_3Cl	63	58.44	.10094	.11375	.12720
Xylene	C_8H_{10}	106	131.60	.06742	.07597	.08495

Source: Shen 1981

See Section 2.3.3 for directions for calculating a final long-term release rate.

(2) Landfills with Internal Gas Generation

Thibodeaux (1981) developed a method for estimating toxic vapor releases from co-disposal landfills. These facilities contain toxic wastes in combination with municipal or sanitary wastes that, because of their considerable organic content, generate landfill gases (e.g., H_2, CH_4, CO_2). In these cases, the upward movement (convective sweep) of the landfill gas becomes the significant controlling factor, greatly accelerating the upward migration and subsequent release to the atmosphere of the co-disposed toxic substances. In fact, review of Thibodeaux's work indicates that the toxic gas migration accelerating the effect of the landfill gas is so great that both soil and gas phase diffusion essentially become insignificant. The following simplified equation is recommended for estimating the volatilization of toxic substances from co-disposal landfills:

$$E_i = C_i^* V_y A \qquad (2\text{-}8)$$

where

E_i = emission rate, (g/sec).
C_i^* = concentration of compound i in the soil pore spaces, (g/cm^3)*
V_y = mean landfill gas velocity in the soil pore spaces, (cm/sec). Thibodeaux (1981) provides an average value of 1.63×10^{-3} cm/sec for this factor.
A = area, (cm^2).

Recalculation of the toxic vapor release estimates presented in Thibodeaux (1981) using this simplified equation yields results within ≃ 1 percent of the values obtained using the full computation cited in the paper. Thibodeaux (1981) notes, however, that various site factors such as the presence of saturated soils will tend to reduce the rate of volatile chemical release from landfills. The degree to which this model is able to accurately reflect contaminant release rates for gases, especially soluble gases, generated at sites with moist or wet soils is unknown.

(3) Spills and Leaks

Equations 2-9 and 2-11 will estimate the volatile releases from fresh and old (respectively) chemical spills on soil. Equations 2-10 and 2-12 through 2-14 provide means of estimating certain input variables required to solve Equations 2-9 and 2-11.

As discussed in Farino et al. (1983), one can apply Equation 2-9 (adapted from Thibodeaux and Hwang 1982) to estimate volatile releases resulting from spills or leaks where a contaminant pool is visible on the soil surface, or where soil is contaminated (saturated) from the surface down. The equation does not consider soil phase mass transfer resistance, and therefore is not appropriate for use when spilled contaminants have seeped into surface soils (in this case, use the landfarming equation that follows). Similarly, because it does not consider liquid phase resistance, it is only useful for estimating releases of pure compounds. The original equation presented in Thibodeaux and Hwang (1982) has been modified to include a contaminated surface area term, thereby resulting in the calculation of a release rate rather than a flux rate value:

$$E_i = k_{iG} C_i^* A \qquad (2\text{-}9)$$

where

E_i = emission rate of chemical i, (g/s).
k_{iG} = gas phase mass transfer coefficient of chemical i, (cm/s).
C_i^* = vapor concentration of chemical i, (g/cm^3).*
A = area, (cm^2).

Hwang (1982) has developed the following simplified means of estimating a compound's gas phase mass transfer coefficient.

$$k_{iG}\left(\frac{MW_{H_2O}}{MW_i}\right)^{0.335}\left(\frac{T}{298}\right)^{1.005}\left(k_{iG},H_2O\right) \qquad (2\text{-}10)$$

where

K_{iG} = gas phase mass transfer coefficient of chemical i, (cm/s).
MW_{H_2O} ; MW_i = molecular weight of water; compound i, (g/mole).
T = temperature, (°K).
k_{iG},H_2O = gas phase mass transfer coefficient for water vapor at 25°C, (cm/sec).

* For conservative analyses, one can assume that the actual contaminant vapor concentration in the soil pore spaces is the same as the equilibrium vapor concentration. In such cases, C_{si} can be used in place of C_i^*. Direct measurements of C_i^*, however, may be developed during the site investigation. When such data are available, their use is preferred.

* For conservative analyses, one can assume that the actual contaminant vapor concentration in the soil pore spaces is the same as the equilibrium vapor concentration. In such cases, C_{si} can be used in place of C_i^*. Direct measurements of C_i^*, however, may be developed during the site investigation. When such data are available, their use is preferred.

When estimating short-term (maximum) release rates, the highest (summer) seasonal temperature expected at the site can be used in calculating the gas phase mass transfer coefficient. For initial estimation of long-term release rates, the seasonal average temperature should be used. Final long-term release notes are developed as discussed in Section 2.3.3.

(4) Landfarming

In cases where past spills, leaks, or intentional disposal directly onto or into surface soils (landfarming) have resulted in contaminated surface soils with liquids in the pore spaces, Equation 2-11 can be used to estimate volatilization releases. This equation assumes that soil pore spaces connect with the soil surface, that soil conditions are isothermal, and that there is no capillary rise of contaminant. It also assumes that there is sufficient liquid contaminant in the pore spaces so that volatilization will not deplete the reservoir of contaminant to the point where it affects the rate of volatilization. Modeling the release from soils with sorbed contaminants and no free liquids requires another model.

Two models for predicting the time-varying volatilization of sorbed contaminants on soil are presented in USEPA (1986e). The equation presented here is adapted from Thibodeaux and Hwang (1982), which presents a volatilization release estimation equation designed for application to active or planned landfarms for petroleum wastes. Farino et al. (1983) determined it to be preferable to other approaches for estimating volatilization release of chemicals spilled or incorporated into soils, because it directly takes into account the contaminant loss over time. It describes vapor diffusion as being soil-phase controlled, and essentially assumes that contaminant concentrations in the soil remain constant (until all contaminant is lost to the air), and that contaminant release occurs by the "peeling away" of successive unimolecular layers of contaminant from the surface of the "wet" (contaminated) zone. Thus, over time this process results in a "dry zone" of increasing depth at the soil surface, and a wet zone of decreasing depth below the dry zone. The original equation has been adjusted somewhat for use at uncontrolled waste sites, and has also been simplified as discussed in Farino et al. (1983), by assuming that the oil layer diffusion length value is low (i.e., that the spilled contaminant has become incorporated into surface soils and is not present as a discrete film).

$$\bar{E}_i = \frac{2DC_sA}{d + \sqrt{\frac{2DC_st}{C_B} + d^2}} \qquad (2\text{-}11)$$

where

- $\bar{E}_i$ = average emission rate of component i over time t, (g/sec).
- D = phase transfer coefficient, (cm^2/sec).
- C_s = the liquid-phase concentration of contaminant i in the soil, (g/cm^3).
- C_B = bulk contaminant concentration in soil (g/cm^3)
- A = contaminated surface area, (cm^2)
- d = depth of dry zone at sampling time, (cm).
- t = time measured from sampling time, (seconds).

D (cm^2/sec) is related to the amount of contaminant i that goes from liquid to gas phase, and then from gas phase to diffusion in air. It can be estimated as follows:

$$D = D_i\left(P_t^{4/3}\right)H_i' \qquad (2\text{-}12)$$

where

- D = phase transfer coefficient, (cm^2/sec).
- D_i = diffusion coefficient of component i in air, (cm^2/sec).
- P_t = total soil porosity, (dimensionless). Again, use of total soil porosity in this equation results in a worst-case (dry soil) estimate for D. As previously discussed, however, in some cases (i.e., where soils are wet more often than dry) it may be more appropriate to use air-filled soil porosity (P_a) in place of P_t. See text addressing Equation 2-3 for a discussion of the application of and values for these two terms.
- H_i' = Henry's Law constant in concentration form, (dimensionless).

H_i', the Henry's Law constant in concentration form (ratio of the boundary layer concentration of contaminant in air to the boundary layer concentration of contaminant in "wet" soil) can be determined as follows (Lyman et al. 1983):

$$H_i' = \frac{H_i}{RT} \qquad (2\text{-}13)$$

where

- H_i = Henry's Law constant of contaminant i, (atm-m^3/mol).
- R = gas constant, (8.2×10^{-5} atm-m^3/mol-°K).
- T = absolute temperature, (°K).

Again, use summer maximum temperatures to estimate short-term release and annual average

temperatures for the initial estimation of long-term release. Final long-term release rates are developed as discussed in Section 2.3.3.

Note that Equation 2-11 assumes that the contaminant concentration in the liquid and gas phases in the soil remains constant until all of the contaminant has been released to air. Also, the equation holds from time zero (the time at which the soil was sampled) to t_d (the time at which the soil becomes dry, i.e., all contaminant has volatilized and the release process stops). The formula for calculating t_d (in seconds) is:

$$t_d = \frac{h^2 - d^2}{2D} \bullet \frac{C_B}{C_s} \qquad (2\text{-}14)$$

where

- t_d = the time at which all contaminant has volatilized from the soil, (sec).
- h = depth from soil surface to the bottom of the contaminated region, (cm).
- d = depth of dry zone at sampling time, (cm).
- D = phase transfer coefficient, (cm^2/sec).
- CB = bulk contaminant concentration in soil, (g/cm^3)
- C_s = contaminant liquid phase concentration (g/cm^3)

(5) Lagoons

Mackay and Leinonen (1975) have developed an equation for estimating volatilization releases of low solubility compounds from waterbodies such as hazardous waste lagoons. This is presented as Equation 2-15. Equations 2-16 and 2-17 provide means of calculating certain input parameters required by Equation 2-15. This approach assumes that conditions are steady state (i.e., no constant addition of contaminant), that diffusion is liquid state controlled, and that it occurs from a well-mixed water phase to a well-mixed air phase across a stagnant water/air interface. As pointed out in Farino et al. (1983), if it can be assumed that atmospheric background levels of the contaminant of concern are negligible, (as would usually be the case at abandoned hazardous waste facilities), then Mackay and Leinonen's basic equation can be simplified to the following form (which includes an area term to convert flux rate to emission rate):

$$E_i = K_i C_s A \qquad (2\text{-}15)$$

where

- E_i = emission rate, (g/sec).
- K_i = overall mass transfer coefficient, (cm/sec).
- C_s = contaminant liquid phase concentration, (g/cm^3)
- A = area, (cm^2).

The overall mass transfer coefficient (K_i) can be calculated via the following relationship:

$$\frac{1}{K_i} = \frac{1}{k_{iL}} + \frac{RT}{H_i k_{iG}} \qquad (2\text{-}16)$$

where

- K_i = overall mass transfer coefficient, (cm/sec).
- k_{iL} = liquid phase mass transfer coefficient, (cm/sec). See Equation 2-17.
- R = ideal gas law constant, (8.2×10^{-5} atm-m^3/mol-°K).
- T = temperature, (°K).
- H_i = Henry's Law constant of compound i, (atm-m^3/mol).
- k_{iG} = gas phase mass transfer coefficient, (cm/sec). See Equation 2-10.

Hwang (1982) provides a simplified method for determining a compound's liquid phase mass transfer coefficient for use in the above equation. To estimate k_{iL}, use the following equation:

$$k_{iL} = \left(\frac{MW_{O_2}}{MW_i}\right)^{0.5} \left(\frac{T}{298}\right) \left(k_{L,O_2}\right) \qquad (2\text{-}17)$$

where

- k_{iL} = liquid phase mass transfer coefficient, (cm/sec).
- MW_{O_2};MW_i = molecular weight of oxygen; compound i.
- T = temperature, (°K).
- k_{L,O_2} = liquid phase mass transfer coefficient for oxygen at 25°C, (cm/sec).

The value for k_{L,O_2} can be obtained from chemical reference texts or can be calculated (the preferred method) as described in Farino et al. (1983).

2.3.2.2 In-Depth Analysis

In-depth analysis of volatile release can be executed in the same manner as that described for particulates. Subtract the monitored upwind (control) ambient toxic vapor concentration from the monitored downwind concentration. Use the difference between these two values in an air dispersion model to estimate the release rate at a "virtual point source" that would correspond with the source of the measured downwind concentration.

The user of this manual should again refer to USEPA (1983c) and Seely et al. (1983) for detailed discussions of the planning and execution of air monitoring studies. Refer to Chapter 3 of this manual

for a description of air contaminant dispersion modeling tools.

2.3.3 Long-Term and Short-Term Release Calculation

Long-term release values (70 years) for lagoons with dilute solutes can be estimated as follows:

$$E_{Ai} = \frac{V_c C_i}{70}\left(1 - e^{-\frac{E}{V_c C_i}(2.2x10^9)}\right) \qquad (2\text{-}18)$$

where

- E_{Ai} = average annual release of contaminant i, (g/yr).
- V_c = volume of contaminated region, (cm^3).
- C_i = initial average concentration of contaminant i in site soils, (g/cm3).
- e = 2.71828
- E = initial combined release rate of contaminant i, (g/sec). Obtained by summing all above-listed releases of the contaminant at the site. For particulates, convert the average annual release from Equation 2-18 to mass per second by dividing by 3.16 x 10^7 seconds.

Note that V_c and C_i must be based on the same value. ($V_c C_i$) is equal to the total mass of contaminant; it can be the total mass of contaminant in a lagoon.

For landfills and wind erosion of contaminated particulates, the release rate is assumed constant. The 70-year average annual release rate can be calculated by first ascertaining if contaminant will remain after 70 years. If so, then the release rate itself is the 70-year average annual release rate. If not, then the 70-year average annual release rate is the total initial mass divided by 70 years.

To estimate long-term release from contaminated surface soils, Equation 2-14 (converted to years by dividing by 3.16 x 10^7) is first used to determine the dry-out time. If no contaminant is expected to remain after 70 years (i.e., 70 > t_d), simply determine the total amount of contaminant present at the time of site investigation and divide by 70 years (in seconds) to get a conservative long-term release value (i.e., $AC_s(h - d)/2.21 \times 10^9$). If some contaminant is expected to remain after 70 years (i.e., 70 < t_d), use the following equation to estimate long-term release:

$$E_{Ai} = \frac{AC_s}{70}\left((d^2 + 4.4 \times 10^9 \frac{C_s}{C_B} D)^{1/2} - d\right) \qquad (2\text{-}19)$$

where

- E_{Ai} = average long-term release of contaminant i, (g/yr).
- A = contaminated area, (cm^2).
- C_s = liquid phase concentration of contaminant i, (g/cm^3).
- d = depth of dry zone at sampling time, (cm).
- D = the amount of contaminant that goes from liquid to gas phase, and then from gas phase to diffusion in air (see Equation 2-12).
- C_B = bulk contaminant concentration in soil (g/cm^3)

Note that this approach does not include consideration of contaminant loss caused by chemical degradation, and thus is conservative in nature.

Finally, for each chemical, sum the long-term volatilization release values from each on-site source to arrive at an overall long-term volatilization release for each contaminant of concern.

Short-term maximum contaminant releases from an uncontrolled hazardous waste facility can be due to a variety of factors. For example, high summer temperatures, ambient pressures, rainfall, and breezy conditions can significantly effect the rate of volatile release, while high winds alone can greatly increase the amount of contaminated particulate matter being blown from the site. Therefore, short-term maximum contaminant release is defined as that level of release calculated for release events during the first one-year period following site investigation.

The above approach to estimating long-term air releases is inherently conservative in that it does not consider site contaminant loss from other (non-air transport) processes. Also, note that the short-term and long-term release values developed in this section will be used, along with worst-case (short-term) and average (long-term) meteorological data, to develop short-term and long-term ambient concentration values for later use in determining exposure levels (see Chapter 3).

2.4 Quantitative Analysis of Surface Water Contamination

Contaminated runoff, overland flow of toxic contaminants from storage leaks and spills, or lagoon failures will often constitute the sources of concern for surface water contamination at uncontrolled hazardous waste sites. Projecting release rates for such contaminant sources can be very difficult, however. Releases from containers or impoundments can best be determined by on-site monitoring of each source. If this is not possible, engineering judgment, combined with a detailed evaluation of site conditions, may provide a basis for developing release estimates. Releases by overland flow of

toxics can be quantified directly by measuring (sampling) the source material and determining the volume and rate of release. Alternatively, runoff release estimation procedures, less costly than monitoring or modeling approaches, can also be applied to uncontrolled sites.

In addition, surface waters may be contaminated by inflows of ground water through bank seepage and springs. In order to estimate the rate of such inflows, one must conduct modeling of ground-water/surface water linkages (see Chapter 3 for a discussion of ground-water modeling options).

This section reviews methods for estimating toxic releases of uncontrolled hazardous waste sites to surface waterbodies. Note, however, that only the surface runoff component of release to surface water is addressed here. Other sources must be estimated for each site based on judgment and experience.

2.4.1 Beginning Quantitative Analysis

2.4.1.1 Dissolved and Sorbed Contaminant Migration

Many of the organic substances of concern found at Superfund sites are relatively nonpolar, hydrophobic substances (Delos et al., 1984). Such substances can be expected to sorb to site soils and migrate from the site more slowly than will polar compounds. As discussed in Haith (1980) and Mills et al. (1982), estimates of the amount of hydrophobic compounds released in site runoff can be calculated using the Modified Universal Soil Loss Equation (MUSLE) and sorption partition coefficients derived from the compound's octanol-water partition coefficient. The MUSLE allows estimation of the amount of surface soil eroded in a storm event of given intensity, while sorption coefficients allow the projection of the amounts of contaminant carried along with the soil, and the amount carried in dissolved form.

(1) Soil Loss Calculation

Equation 2-20 is the basic equation for estimating soil loss. Equations 2-21 through 2-24 are used to calculate certain input parameters required to apply Equation 2-20. The modified universal soil loss equation (Williams 1975), as presented in Mills et al. (1982), is:

$$Y(S)_E = a(V_r q_p)^{0.56}\, KLSCP \qquad (2\text{-}20)$$

where

- $Y(S)_E$ = sediment yield (tons per event, metric tons per event).
- a = conversion constant, (95 English, 11.8 metric).*
- V_r = volume of runoff, (acre-feet, m^3).
- q_p = peak flow rate, (cubic feet per second, m^3/sec).
- K = the soil erodibility factor, (commonly expressed in tons per acre per dimensionless rainfall erodibility unit). K can be obtained from the local Soil Conservation Service office.
- L = the slope-length factor, (dimensionless ratio).
- S = the slope-steepness factor, (dimensionless ratio).
- C = the cover factor, (dimensionless ratio: 1.0 for bare soil; see the following discussion for vegetated site "C" values).
- P = the erosion control practice factor, (dimensionless ratio: 1.0 for uncontrolled hazardous waste sites).

Soil erodibility factors are indicators of the erosion potential of given soil types. As such, they are highly site-specific. K values for sites under study can be obtained from the local Soil Conservation Service office. The slope length factor, L, and the slope steepness factor, S, are generally entered into the MUSLE as a combined factor, LS, which is obtained from Figures 2-4 through 2-6. The cover management factor, C, is determined by the amount and type of vegetative cover present at the site. Its value is "1" (one) for bare soils. Consult Tables 2-4 and 2-5 to obtain C values for sites with vegetative covers. The factor, P, refers to any erosion control practices used on-site. Because these generally describe the type of agricultural plowing or planting practices, and because it is unlikely that any erosion control would be practiced at an abandoned hazardous waste site, use a worst-case (conservative) P value of 1 (one) for uncontrolled sites.

Storm runoff volume, V_r, is calculated as follows (Mills et al. 1982):

$$V_r = aAQ_r \qquad (2\text{-}21)$$

where

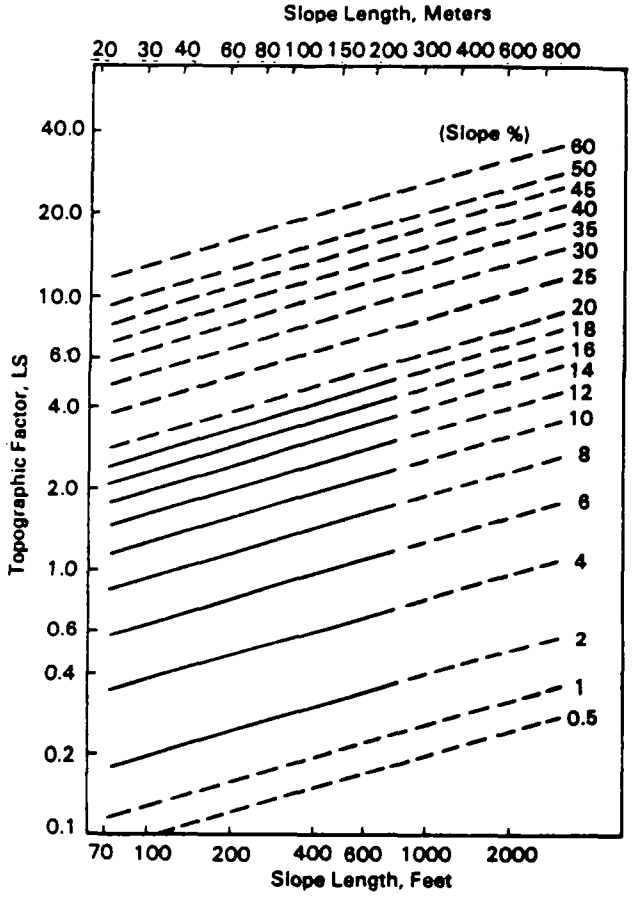
- a = conversion constant, (0.083 English, 100 metric).
- A = contaminated area, (acres, ha).
- Q_r = depth of runoff, (in, cm).

Depth of runoff, Qr, is determined by (Mockus 1972):

$$Q_r = (R_t - 0.2S_w)^2/(R_t + 0.8S_w) \qquad (2\text{-}22)$$

* Metric conversions presented in the following runoff contamination equations are from Mills et al. (1982).

Figure 2-4. **Slope effect chart applicable to areas A-1 in Washington, Oregon, and Idaho, and all of A-3: see Figure 2-5 (USDA 1974 as presented in Mills et al. 1982).**



NOTE: Dashed lines are extension of LS formulae beyond values tested in studies.

where

R_t = the total storm rainfall, (in, cm).
S_w = water retention factor, (in, cm).

The value of S_w, the water retention factor, is obtained as follows (Mockus 1972):

$$S_w = \frac{1000}{CN} - 10\,a \qquad (2\text{-}23)$$

where

S_w = water retention factor, (in, cm).
CN = the SCS Runoff Curve Number, (dimensionless, see Table 2-6).
a = conversion constant (1.0 English, 2.54 metric).

The CN factor is determined by the type of soil at the site, its condition, and other parameters that establish a value indicative of the tendency of the soil to absorb and hold precipitation or to allow precipitation to run off the surface. The analyst can obtain CN

Figure 2-5. **Soil moisture-soil temperature regimes of the western United States (USDA 1974 as presented in Mills et al. 1982).**

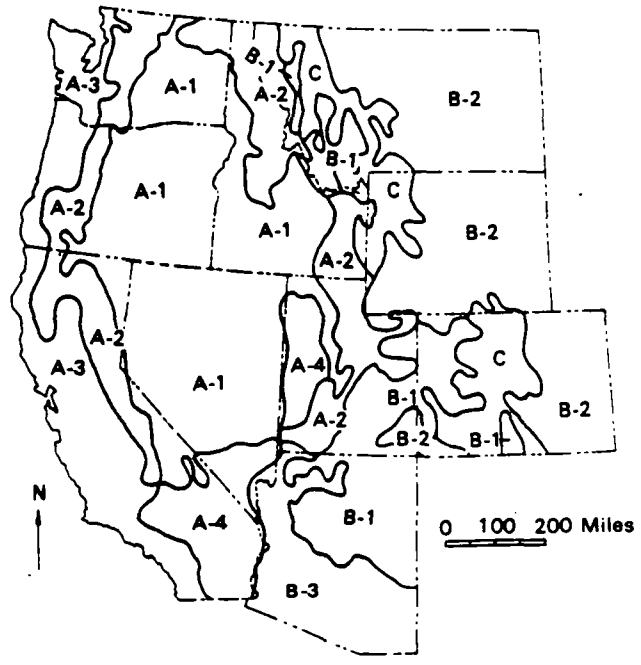
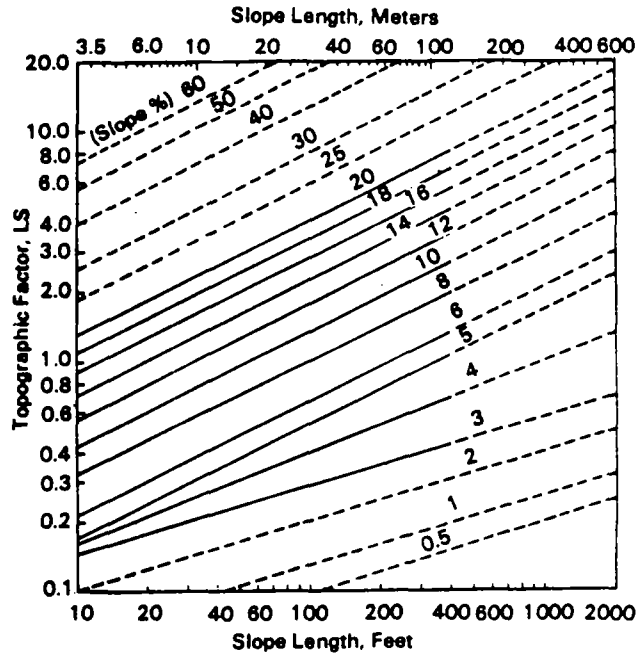


Figure 2-6. **Slope effect chart for areas where Figure 2-5 is not applicable (USDA 1974 as presented in Mills et al. 1982).**



NOTE: The dashed lines represent estimates for slope dimensions beyond the range of lengths and steepnesses for which data are available.

values of uncontrolled hazardous waste sites from Table 2-6.

The peak runoff rate, q_p, is determined as follows (Haith 1980):

$$q_p = \frac{aAr_tQ_r}{T_r(R_t - 0.2S_w)} \qquad (2\text{-}24)$$

where

- q_p = the peak runoff rate, (ft^3/sec, m^3/sec).
- a = conversion constant, (1.01 English, 0.028 metric).
- A = contaminated area, (acres, ha).
- R_t = the total storm rainfall, (in, cm).
- Q_r = the depth of runoff from the watershed area, (in, cm).
- T_r = storm duration, (hr).
- S_w = water retention factor, (in, cm).

(2)Dissolved/Sorbed Contaminant Release
As discussed in Mills et al. (1982), the analyst can predict the degree of soil/water partitioning expected for given compounds once the storm event soil loss has been calculated with the following equations. First, the amounts of adsorbed and dissolved substances are determined, using the equations presented below as adapted from Haith (1980):

$$S_s = [1/(1 + \Theta_c/(K_d\beta))](C_i)(A) \qquad (2\text{-}25)$$

and

$$D_s = [1/(1 + (K_d\beta)/\Theta_c)](C_i)(A) \qquad (2\text{-}26)$$

where

- S_s = sorbed substance quantity, (kg, lb).
- Θ_c = available water capacity of the top cm of soil (difference between wilting point and field capacity), (dimensionless).
- K_d = sorption partition coefficient, (cm^3/g).
- β = soil bulk density, (g/cm^3).
- C_i = total substance concentration, (kg/ha-cm, lb/acre-cm).
- A = contaminated area, (ha-cm acre-cm). (Actually a volume; assumption is contamination in upper 1 cm is available for release.)
- D_s = dissolved substance quantity, (kg, lb).

This model assumes that only the contaminant in the top 1 cm of soil is available for release via runoff.

The soil sorption partition coefficient for a given chemical can be determined from known values of certain other physical/chemical parameters, primarily the chemical's octanol-water partition coefficient, solubility in water, or bioconcentration factor. Lyman et al. (1982) present regression equations that allow the analyst to determine sorption coefficients for specified groups of chemicals (e.g., herbicides, polynuclear aromatics). If parameter values required by the appropriate equations are not available in chemical reference literature, they can be estimated according to procedures described in Lyman et al. (1982). Initially, the octanol-water partition coefficient can be estimated based on the substance's molecular structure. If necessary, this value can be used, in turn, to estimate either solubility in water or bioconcentration factor.

After calculating the amount of sorbed and dissolved contaminant, the total loading to the receiving waterbody is calculated as follows (adapted from Haith 1980):

$$PX_i = [Y(S)_E/100\,\beta]\,S_s \qquad (2\text{-}27)$$

plus

$$PQ_i = [Q_r/R_t]\,D_s \qquad (2\text{-}28)$$

where

- PX_i = sorbed substance loss per event, (kg, lb).
- $Y(S)_E$ = sediment yield, (tons per event, metric tons).
- β = soil bulk density, (g/cm^3).
- S_s = sorbed substance quantity, (kg, lb).
- PQ_i = dissolved substance loss per event, (kg, lb).
- Q_r = total storm runoff depth, (in, cm).
- R_t = total storm rainfall, (in, cm).
- D_s = dissolved substance quantity, (kg, lb).

PX_i and PQ_i can be converted to mass per volume terms for use in estimating contaminant concentration in the receiving waterbody by dividing by the site storm runoff volume (V_r, see Equation 2-21).

2.4.2 In-Depth Analysis

Releases to surface waterbodies at uncontrolled hazardous waste sites can be quantified most accurately by direct measurement (sampling and analysis) of the contaminant flow. Alternatively, upcurrent and downcurrent sampling can be conducted to determine the release level at the site that would be used to estimate the ambient concentration (i.e., the difference between the upcurrent and downcurrent concentrations). Either simple dispersion equations or sophisticated computer modeling approaches (see Chapter 3) can be used to "back calculate" the measured ambient concentration to the "virtual point source."

Table 2-4. "C" Values for Permanent Pasture, Rangeland, and Idle Land

Vegetal canopy Type and height of raised canopy[b]	Canopy cover[c] (%)	Cover that contacts the surface: Type[d]	Percent ground cover: 0	20	40	60	80	95-100
No appreciable canopy		G	0.45	0.20	0.10	0.042	0.013	0.003
		W	0.45	0.24	0.15	0.090	0.043	0.011
Canopy of tall weeds or short brush (0.5 m fall height)	25	G	0.036	0.17	0.09	0.038	0.012	0.003
		W	0.036	0.20	0.13	0.082	0.041	0.011
	50	G	0.026	0.13	0.07	0.035	0.012	0.003
		W	0.026	0.16	0.11	0.075	0.039	0.011
	75	G	0.17	0.10	0.06	0.031	0.011	0.003
		W	0.17	0.12	0.09	0.067	0.038	0.011
Appreciable brush or brushes (2 m fall height)	25	G	0.40	0.18	0.09	0.040	0.013	0.003
		W	0.40	0.22	0.14	0.085	0.042	0.011
	50	G	0.34	0.16	0.085	0.038	0.012	0.003
		W	0.34	0.19	0.13	0.081	0.041	0.011
	75	G	0.28	0.14	0.08	0.036	0.012	0.003
		W	0.28	0.17	0.12	0.077	0.040	0.011
Trees but no appreciable low brush (4 m fall height)	25	G	0.42	0.19	0.10	0.041	0.013	0.003
		W	0.42	0.23	0.14	0.087	0.042	0.011
	50	G	0.39	0.18	0.09	0.040	0.013	0.003
		W	0.39	0.21	0.14	0.085	0.042	0.011
	75	G	0.36	0.17	0.09	0.039	0.012	0.003
		W	0.36	0.20	0.13	0.083	0.041	0.011

Source: Wischmeier 1972

[a]All values shown assume: (1) random distribution of mulch or vegetation, and (2) mulch of appreciable depth where it exists.
[b]Average fall height of waterdrops from canopy to soil surface: m = meters.
[c]Portion of total-area surface that would be hidden from view by canopy in a vertical projection (a bird's-eye view).
[d]G: Cover at surface is grass, grasslike plants, decaying compacted duff, or litter at least 5 cm (2 in) deep.
W: Cover at surface is mostly broadleaf herbaceous plants (as weeds) with little lateral-root network near the surface and/or undecayed residue.

Table 2-5. "C" Values for Woodland

Stand condition	Tree canopy percent of area[a]	Forest litter percent of area[b]	Undergrowth[c]	"C" factor
Well stocked	100-75	100-90	Managed[d]	0.001
			Unmanaged[d]	0.003-0.011
Medium stocked	70-40	85-75	Managed	0.002-0.004
			Unmanaged	0.01-0.04
Poorly stocked	35-20	70-49	Managed	0.003-0.009
			Unmanaged	0.02-0.09[e]

Source: Wischmeier 1972

[a]When tree canopy is less than 20 percent, the area will be considered as grassland or cropland for estimating soil loss.
[b]Forest litter is assumed to be at least 2 in deep over the percent ground surface area covered.
[c]Undergrowth is defined as shrubs, weeds, grasses, vines, etc., on the surface area not protected by forest litter. Usually found under canopy openings.
[d]Managed - grazing and fires are controlled.
Unmanaged - stands that are overgrazed or subjected to repeated burning
[e]For unmanaged woodland with litter cover of less than 75 percent, C values should be derived by taking 0.7 of the appropriate values in Table 3-4. The factor of 0.7 adjusts for much higher soil organic matter on permanent woodland.

Table 2-6. Runoff Curve Numbers

Soil group	Description	Site type: Overall site[a]	Road/right of way	Meadow	Woods
A	Lowest runoff potential: Includes deep sands with very little silt and clay, also deep, rapidly permeable loess (infiltration rate = 8-12 mm/h).	59	74	30	45
B	Moderately low runoff potential: Mostly sandy soils less deep than A, and loess less deep or less aggregated than A, but the group as a whole has above-average infiltration after thorough wetting (infiltration rate = 4-8 mm/h).	74	84	58	66
C	Moderately high runoff potential: Comprises shallow soils and soils containing considerable clay and colloids, though less than those of group D. The group has below-average infiltration after presaturation (infiltration rate = 1-4 mm/h).	82	90	71	77
D	Highest runoff potential: Includes mostly clays of high swelling percent, but the group also includes some shallow soils with nearly impermeable subhorizons near the surface (infiltration rate = 0-1 mm/h).	86	92	78	83

Source: Adapted from Schwab et al. 1966.
[a]Values taken from farmstead category, which is a composite including buildings, farmyard, road, etc.

2.4.3 Long-Term and Short-Term Release Calculation

For surface runoff releases, the long-term release value can be calculated as follows:

- Characterize an average storm event for the area in terms of duration. This can best be accomplished by consulting local or regional climatological experts, or the National Climatological Data Center in Asheville, North Carolina. Then, using USDC (1961), determine the amount of rainfall corresponding to the selected duration rainfall event on a one year-return frequency basis. Divide this amount into the mean annual rainfall for the area to obtain the average number of average rainfall events per year.

- Use these data and the equations presented in this section to calculate runoff contaminant release associated with each yearly average storm.

- Estimate the potential total long-term release for both dissolved and sorbed runoff loss* as follows:

$$E_{Ai} = BN \qquad (2\text{-}29)$$

where

E_{Ai} = long-term release of contaminant i in runoff, (mass/70 years).
B = dissolved or sorbed loss per storm event, (i.e., PX_i or PQ_i; see Equations 2-27 and 2-28).
N = number of "average" storm events in 70 years.

- Determine the total amount of soil that will erode from the site over 70 years. This can be accomplished by applying the Universal Soil Loss Equation (USLE-Wischmeier and Smith 1978). This equation, from which the MUSLE (see Equation 2-20) was developed, estimates annual soil losses in runoff. The USLE takes the same form as the MUSLE, except that the storm event-specific volume and flow rate variables are replaced by a factor, R, the rainfall runoff factor. Therefore, the USLE is:

$$Y(S)_A = R_r KLSCPAS_d \qquad (2\text{-}30)$$

where

$Y(S)_A$ = annual soil loss in runoff, (tons/yr, tonnes/yr).

* This approach is overly conservative as it assumes that the contaminant concentration in surface soil remains essentially the same during the entire 70-year period.

R_r = the rainfall and runoff factor, expressing the erosion potential of average annual rainfall in the locality (can be obtained from the local Soil Conservation Service office), (dimensionless).

K = the soil-erodibility factor, commonly expressed in tons per acre per R_r unit (can be obtained from the local Soil Conservation Service office) (in metric tons/ha/R_r unit), (English K*1.292 = metric K).

L = the slope length factor, (dimensionless).

S = the slope steepness factor, (dimensionless).

C = the cover factor, (dimensionless ratio: 1.0 for soil, see the following discussion for vegetated site "C" values).

P = the erosion control practice factor, (dimensionless: 1.0 for uncontrolled hazardous waste sites).

A = acreage of area, (acres, ha).

S_d = the sediment delivery ratio, (dimensionless).

The sediment delivery ratio (S_d) can be estimated using the following equation:

$$S_d = D_d^{-0.22} \qquad (2\text{-}31)$$

where

D_d = the overland distance between the site and the receiving waterbody (ft).

Mills et al. (1982) note that this equation was empirically derived from data for D values from 0 to 800 feet, and caution that it may require further testing, particularly in sites located in the Midwest and Central U.S.

Note that in certain areas of the Pacific Northwest and central western states, thaw and snowmelt may contribute most of the runoff erosive force on an annual basis. In such cases, an additional erosion factor, R_s, must be added to the rainfall and runoff factor, R, to calculate the total R value for use in the USLE. Limited field data have indicated that an approximate estimate of R_s may be obtained by multiplying 1.5 times the local average total rainfall (in inches) for the period December 1 through March 31 (Wischmeier and Smith 1978). However, the local Soil Conservation Service office can provide the overall R value (R_r plus R_s).

- Based on site monitoring data, estimate the average contaminant concentration in the layer of soil that must be eroded to equal the total estimated amount of soil lost over 70 years (based on site soil sampling data and the calculated vertical depth of soil that will erode over that time period).

- Multiply the average contaminant concentration on site by the site area to calculate the mass of contaminant present in that amount of soil estimated to be eroded over 70 years. This represents the maximum amount of contaminant available for erosion losses over the 70-year period.

- Compare the estimated potential contaminant runoff losses over 70 years with the mass of contaminant present (in 70-year erodible soils at the site). If the estimated total loss to runoff is less than the amount available, divide the estimated total 70-year losses by the total volume of stormwater runoff estimated over 70 years. This will approximate the contaminant concentration in runoff (both dissolved and sorbed).

- If the total estimated contaminant runoff losses exceed the amount of contaminant present in 70-year erodible site soils, divide the total mass of contaminant present in such soils by the volume of runoff estimated to leave the site over 70 years to develop adsorbed and dissolved contaminant loss estimates in concentration form. In either case, the runoff value needed to estimate contaminant transport and dispersion in surface waterbodies can be estimated by dividing the total volume of runoff estimated to leave the site over 70 years by the number of seconds, minutes, etc. in 70 years to estimate runoff volume per unit time.

Many factors can influence the actual degree of contaminant loss in given storm events. Because such factors vary from locale to locale, no single method will guarantee accurate estimates of short-term contaminant losses in runoff from all sites. However, the following approach should yield reasonable approximations of the magnitude of such short-term loss. While short duration, high intensity storm events (thunderstorms) clearly cause significant erosion, the water quality effects of such storms are too ephemeral to adequately reflect short-term releases as defined (i.e., 10 to 90 days). Therefore, a storm event is needed that will generate contaminant releases adequate to affect water quality over a time period approaching the 10-day lower bound of the short-term time frame. For this analysis, a 1-year, 24-hour storm event has been selected. Data quantifying the amount of rainfall that corresponds to the 1-year, 24-hour storm event (as well as similar data for other storm return periods and durations) are provided in USDC (1961). To estimate short-term runoff release, the average site contaminant concentration should be estimated based on sampling

data for the top cm of soil only. This value is then used in Equations 2-27 and 2-28 to estimate runoff losses on a single storm event basis.

Research based on the work of Haith et al. (1980) is currently underway at Cornell University* to develop runoff loading factors for organic chemicals in soils. After these factors are devised, the analyst will be able to obtain average loading values based solely on a chemical's octanol/water partition coefficient and the geographic location under study. This will greatly simplify the generation of long-term average release estimates.

Note that in order to estimate long-term and short-term contaminant concentrations in surface water, the long-term and short-term release values are used, along with average and minimum streamflow data as described in Chapter 3, Environmental Fate Analysis.

2.5 Quantitative Analysis of Ground-Water Contamination

Surface soils at uncontrolled hazardous waste sites may become contaminated with toxic materials as a result of (1) the intentional placement of wastes on the ground (dumping, landfarming), (2) spills, (3) lagoon failure (overland flow), or (4) contaminated site runoff. Leaching of toxics from a contaminated soil surface can carry contaminants into subsurface layers.

2.5.1 Beginning Quantitative Analysis

2.5.1.1 Leachate Release Rate

This section presents simplified approaches for estimating contaminant release rates to ground water. Such estimation can be determined for dry landfills, lagoons, or wet landfills, whether unlined or lined with clay or flexible membrane liners.

(1) Estimating Release Rate from Facilities Lined with Clay or Natural Soil

Release rate estimation involves the determination of both the contaminant concentration in the leachate and the volumetric flux of leachate. The determination of contaminant concentration is made using equilibrium conditions (steady state), whereas the volumetric flux can be ascertained with instantaneous time-varying models or with steady state equations.

Modeling the release rate of toxic constituents can thus be done in terms of either the instantaneous time-varying releases or the annual average release (i.e., steady state release rate based on an annual average). This section discusses the determination of the steady state release rate (annual average); the equations are simpler than the computer models necessary for instantaneous time-varying releases. Analysts interested in performing instantaneous time-varying release rate determinations are referred to Chapter 3, where the HELP and SESOIL models are discussed. HELP and SESOIL are appropriate for modeling dry solid waste in a landfill or landfarm situation; they are not appropriate for modeling the release rate of liquids from lagoons, landfills, or landfarms. Rainstorms come in discrete intervals separated by dry periods. Using steady state equations to model rainfall-induced leaching, however, assumes that 1/365th of the annual recharge occurs each day. Although this is an assumption, it is felt to be a useful one for most cases. Most abandoned hazardous waste sites have received liquids in the past; very few have received only dry solids. Hence, the question of the assumption of steady state conditions is relatively moot. For the bulk of the modeling situations (liquid wastes), the steady state and the instantaneous rates are the same, and since the steady state equations are simpler, they are the method of choice.

For lagoons, the analyst should use the concentration of contaminant in the lagoon as the concentration of the contaminant leaving the lagoon, since the "leachate" is the waste itself. The waste leaves the lagoon by percolating through the clay liner or the native soil, or it permeates the flexible membrane liner (FML).

For landfills, the analyst should use the equilibrium solubility of the solid waste, assuming that the contaminant will have fully equilibrated with the percolating rainwater. The use of the equilibrium solubility concentration as the leachate concentration is an assumption, it is based on a typical residence time of 21 years for rain percolating through a covered (10^{-7} cm/sec) secure landfill. The assumption is that the time used for determining the equilibrium solubility of the chemical is much shorter than the residence time in the fill. If the fill is uncovered (or covered with a permeable cover), the travel time through the landfill may be too short for the above assumptions to be valid. In these cases, the analyst should calculate the travel time and compare it to the time used in the solubility test. If the travel time is not longer than the test time, the analyst should estimate the leachate concentration as a fraction of the equilibrium solubility concentration. Additionally, the above assumptions assume a landfill of only one waste stream, if the fill has only a small quantity of the subject waste in it, the contact time is the time for travel through the isolated material. In these conditions, the leachate concentration will typically be a fraction of the equilibrium solubility. The analyst may wish, in some instances, to model the solubility of the contaminant within a complex leachate. In this case, the solubility of a hydrophobic

* Contact Douglas A. Haith, Cornell University, Ithaca, N.Y., (607)256-2280.

contaminant can be increased by the organic fraction of the complex leachate.

For landfarms, the assumption that adequate residence time is available for contaminants to reach equilibrium solubility may not be viable, and the analyst should estimate the degree of solubilization. This can be done by dynamic modeling of the kinetics of dissolution, or it can be approximated based on experience and engineering judgment. Because of the complexities of dynamic modeling, this approach usually is not worth the slightly increased accuracy gained, especially since other parameters may affect the accuracy of the final answer. Concentration is typically estimated as a fraction of the equilibrium solubility.

The volumetric flux of contaminated water can be calculated in two ways, one for solid wastes and one for liquid wastes.

(a) For landfilled solids, the only liquid present is water percolating into the fill. For uncovered landfills, this can range from the infiltration fraction of the rainfall, to the full precipitation (if no rain runs off of the fill before infiltrating), to larger flows of water if the site is exposed to stormwater run-on from an adjacent area. For covered landfills, the infiltration fraction may be limited by the permeability of the cover. Typically in wet climates the cover permeability is limiting, while in dry climates the permeability does not limit percolation, and normal soil percolation ratios can be used.

The loading rate to ground water can be calculated with the following equation:

$$L_c = q * A * C_o \qquad (2\text{-}32)$$

where

- L_c = contaminant loading rate, (mass/time).
- q = percolation rate, see Equation 3-14 for calculation of q, (length/time).
- A = area of landfill, (length squared).
- C_o = solubility of solid chemical, (mass/volume).

(b) For lagooned or landfilled liquids, precipitation has a minimal influence on leachate generation, as liquid waste will percolate to the watertable under the influence of gravity. The rate-determining step is the permeability of the liner or underlying soil (if there is no liner). For liquids, the following form of Darcy's law should be used to estimate the volumetric flux leaving the site.

$$Q_l = K_s * i * A \qquad (2\text{-}33)$$

where

- Q_l = volume loading rate, (volume/time).
- K_s = Darcy's coefficient; for unlined lagoons use native soil hydraulic conductivity; conductivity (length/time) (see Chapter 3 for sources of hydraulic conductivity).
- i = hydraulic gradient, (length/length). Equations 2-33 will handle situations where the liquids in the lagoon have a free depth. In many cases the depth of the free liquids is small, or it is small with respect to the distance between the lagoon and the watertable (when the Ks is for native soil). In these cases the term "i" can be taken as 1.
- A = area of lagoon, (length squared).

This Q_l is then used to estimate mass loadings with the following equation:

$$L_c = C_s * Q_l \qquad (2\text{-}34)$$

where

- L_c = contaminant loading rate, (mass/time).
- C_s = contaminant concentration in lagoon fluid, (mass/volume).
- Q_l = volume loading rate, (volume/time).

Equations 2-33 and 2-34 model the release rate from a lagoon whether the flow through the vadose zone is saturated or unsaturated. For unlined active lagoons, the flow is typically saturated all the way to the watertable. For clay-lined lagoons, the flow is saturated through the liner and unsaturated between the liner and the watertable (assuming no breaches in the liner). Equations 2-33 and 2-34 are appropriate when analyzing lagoon releases, but should not be used for spills or other conditions where the chemicals on the surface do not pond for a long time. In these conditions, the assumption of saturated flow (through the liner or soil) may be violated.

Equations 2-33 and 2-34 apply to liquids that are mostly water. For lagoons that contain organic fluids, however, the equations may need to be corrected. For liquids with a density or viscosity that differs from water, correct K_s for this different viscosity and density by calculating the term K_c, using the following:

$$K_c = K_w * D_c/D_w * u_w/u_c \qquad (2\text{-}35)$$

where

- K_c = corrected K_s term = hydraulic conductivity of contaminant, (length/time).
- K_w = hydraulic conductivity of ground water, (length/time).
- D = density of liquids: c = contaminant, w = water, (mass/volume).

u = dynamic viscosity of liquids: c = contaminant, w = water, (mass/length * time).

and then substituting K_c for K_s in Equation 2-33.

(2) Estimating Release Rate from Facilities Lined with Flexible Membranes

The release rate from an intact lined landfill or lagoon can be calculated for a small group of contaminants. Failed liners can be modeled as a function of the extent of the failure using the modeling equations for clay or natural soil-lined facilities. Although a flexible membrane (FML) liner appears to allow no migration through the barrier, it may indeed be penetrated by organic compounds and contaminated water, although the rate of permeation is understandably small. The rate at which a contaminant permeates through a polymeric material has been shown to be dependent upon various properties of the permeant, such as size, shape, polarity, and other factors (Steingiser et al. 1978).

Salame and others proposed the use of a permeability equation to predict the rate of permeation of liquids and gases through various polymers (Salame 1961, 1973, 1985; Steingiser et al. 1978):

$$P_s = A_p \varnothing e^{-S_H} \qquad (2\text{-}36)$$

where

P_s = permeation rate, (g-mil/100 in^2*day*cmHg).
A_p = constant solely dependent on the type of polymers used, (g-mil/100 in^2*day*cmHg).
S_H = constant solely dependent on the type of polymers used, (cc/cal).
$\varnothing$ = the polymer "permachor" calculated for each polymer-permeant pair, (cal/cc).

Salame lists values for these parameters obtained from his extensive experimental work. These values are shown in Tables 2-7, 2-8, 2-9, and 2-10.

For permeation of water through FMLs, polymers are categorized into five groups based on the values of the solubility parameter as shown in Table 2-8. This grouping was achieved after examination of experimental data for about 70 different polymers (Salame 1985). The solubility parameter provides an indication of polymer interaction with water, with more interaction occurring at higher values of the solubility parameter. Examples of hydrogen bonding for polymer group 5 include hydroxyl (OH) and amide (NHCO) radicals as in nylon and polyvinyl alcohol. The polymer with hydrogen bonding but with the value of "delta" less than 11 does not belong to group 5. Permachor values for some selected organic liquids and for water are shown in Tables 2-9 and 2-10, respectively. The water "permachor" values for various polymers given in Table 2-10 apply under dry conditions. For water permeation under wet conditions, permachor values may be reduced by about 20 percent.

The term P can be used to calculate the release rate in grams/day. P is multiplied by the area of the liner, and then divided by its thickness. This assumes a normal water vapor pressure of 1 cm Hg at ambient temperature. The equation is:

$$L_c = P_s * A * p / d_l \qquad (2\text{-}37)$$

where

L_c = contaminant loading rate, (mass/time).
P_s = permeation rate, (g-mil/100 in^2*day*cmHg).
A = area of liner, (in units of 100 in^2).
p = vapor pressure, (cmHg).
d_ℓ = thickness of the liner, (mils).

2.5.2 *In-Depth Analysis*

In-depth analytical approaches for quantification of baseline contaminant release to ground water involve the use of computerized models. Refer to Chapter 3 of this manual for a detailed discussion of the nature and applications of such modeling tools.

2.5.3 *Long-Term and Short-Term Release Calculation*

For toxic substance release to ground-water systems, directly calculate the short-term (maximum) release values from the measured surface and subsoil contaminant concentrations using the tools discussed in this section. Obtain long-term (average) values by applying the procedure previously outlined for particulate releases to air (see Section 2.3.3).

2.6 Soil Contamination

2.6.1 *Beginning Quantitative Analysis*

No estimation methods are presented for analysis of surface soil contamination. Site soils will be sampled directly and the degree and extent of their contamination delineated during the Remedial Investigation. Sampling and analysis may also have been conducted for subsurface soils. In certain cases, however, it may be desirable to project subsurface contamination without conducting unsaturated zone sampling. USEPA (1987a) covers soil sampling strategies.

2.6.2 *In-Depth Analysis*

Surface soil monitoring, usually conducted during the Remedial Investigation, constitutes in-depth quantitative analysis. Subsurface (unsaturated zone) in-depth analysis will usually involve application of sampling and modeling approaches. Sampling and

Table 2-7. Parameter Values for Permeation Equation (at 25°C)

Parameter	Liquid organics in[a]		Water in polymer category[b]				
	PE	NVC	1	2	3	4	5
A $\frac{\text{g-mil}}{100\ \text{in}^2\ \text{day cmHg}}$	1×10^4	1×10^4	11.5	10.2	5.4×10^2	25	(d)
s (cc/cal)	0.506	0.23	0.16	0.135	0.115	0.035	0.099
Ø(cal/cc)	Table 2-9[c]			Table 2-10[c]			

[a]Source: Salame n.d.; Salame 1961.
[b]See Table 2-8 regarding polymer category. Source: Salame 1985.
[c]See the table indicated for these values.
[d]$A \approx 0.33 \exp(0.064 \times \sigma^2)$, where σ is the solubility parameter, $(\text{cal/cc})^{1/2}$.

Table 2-8. Polymer Categorization for Permeation of Water

Polymer group	Categorization
1	Any polymer with $\delta < 8.9$a
2	Any polymer with $8.9 < \delta < 10$
3	Any polymer with $10 < \delta < 11$
4	Polymer containing nitrile (CN) group with $10.5 < \delta$
5	Polymer with H bonding and $11 < \delta$

[a]δ = Solubility parameter $(\text{cal/cc})^{1/2}$
Source: Salame 1985.

analysis can provide a direct quantification of the degree of contamination in subsurface soils. Alternatively, computer models (e.g., SESOIL; Bonazountas and Wagner 1981) are used to project the level of unsaturated zone contamination over time from surface placement of toxics. Refer to Chapter 3 of this manual for a detailed discussion of computer models that can be applied to the unsaturated zone contamination estimation.

Table 2-9. Permachor Values of Some Organic Liquids in Polyethylene and PVC[a]

Liquid	In nonpolar polymer Ø	In polar polymer Ø
Acetic acid	13.0	44.0
Benzaldehyde	15.9	4.0
Benzene	5.4	7.0
2-Butoxy ethanol	24.4	75.0
Butyl acetate	13.0	5.0
Butyl alcohol	18.0	50.0
Butyl ether	10.4	46.0
Butyraldehyde	13.5	0.0
Caprylic acid	19.0	50.0
Carbon tetrachloride	5.8	22.0
p-chlorotoluene	7.6	7.5
Cyclohexane	7.0	45.0
Dibutylphthalate	31.4	17.0
Diethylamine	10.0	5.7
Ethanol	16.0	48.0
Heptane	7.0	44.0
Hexane	6.0	43.0
Methyl ethyl ketone	12.5	1.0
Methanol	15.0	47.0
Nitroethane	15.4	7.0
i-Pentyl propionate	15.0	7.0
i-Propyl amine	11.0	6.7
Trichloroethylene	5.4	3.0
o-Xylene	9.4	11.0
p-Xylene	7.4	9.0

[a]Polyethylene and PVC are nonpolar and polar polymers, respectively.
Sources: Salame n.d.; Steingiser et al. 1978.

Table 2-10. Water Permachor Value for Dry Polymers

Polymer	Permachor value (Ø)
Polyvinyl alcohol	160
Polyacrylonitrile	109
Cellulose (dry)	97
Polyvinylidene chloride	87
Polycaprolactam (dry)	80
Polyacrylonitrile styrene (70/30) (Lopac)	76
Polyacrylonitrile styrene/butadiene (70/23/7) (Cycopac930)	75
Polychlorotrifluoroethylene	71
Polyethylene terephthalate	68
Polyvinylidene fluoride (Kynar)	67
Polyacrylonitrile styrene/ = a/butadiene (56/27/4/13) (Cycopac 920)	65
Polyvinyl chloride	62
Polyoxymethylene (Delrin)	57
Polymethyl methacrylate	55
Polyvinyl acetate (dry)	45
Polystrene/acrylonitrile (74/26)	45
Polyethylene (HD)	40
Polysulfone	34
Polypropylene	33
Polycarbonate (Lexan[3])	33
Polystyrene	28
Polyethylene (LD)	26
Polyisobutylene	17
Polyethylene/vinyl acetate (85/15)	15
Polybutadiene	8
Polymethyle pentene (TPX)	8
Polydimethyl siloxane (dry)	-4

Sources: Salame 1961; Salame n.d.; Staingiser et al. 1978.

Chapter 3
Contaminant Fate Analysis

3.1 Introduction

This chapter provides guidance for evaluating the transport, transformation, and fate of contaminants in the environment following their release from an uncontrolled hazardous waste site. The contaminant release rate estimates described in the previous chapter provide the basis for contaminant fate analysis. The results form the basis for subsequent analysis of exposed populations and estimation of the levels of exposure incurred (see Appendix A). The goal of contaminant fate analysis is to identify off-site areas affected by contaminant migration and to determine contaminant concentrations in these areas.

The following sections address analysis of atmospheric fate, surface water fate, ground-water fate, and biotic fate. Within each of those sections, contaminant transport is addressed (except for biotic fate analysis, which does not involve contaminant transport). A screening analysis is conducted to provide an initial qualitative assessment of contaminant transport in the environment. It is designed to (1) identify each transport process governing the movement of various contaminants within and among environmental media, (2) determine the direction and roughly gauge the rate of contaminant movement from the site, and (3) identify areas to which contaminants have been or may be transported. Screening analysis is designed both to provide initial organization and direction for subsequent in-depth analysis of contaminant environmental transport, and to provide a consistent basis for analysis from site to site.

When likely pathways of contaminant migration have been identified by screening analysis, those pathways requiring further evaluation are quantitatively addressed. Like analysis of contaminant release, this analysis can involve either the use of "desktop" analytical solutions or numeric methodology.

Simplified environmental fate estimation procedures are based on the predominant mechanisms of transport within each medium, and they generally disregard intermedia transfer or transformation processes. In general, they produce conservative estimates (i.e., reasonable upper bounds) for final ambient concentrations and the extent of hazardous substance migration. However, caution should be taken to avoid using inappropriate analytical methods that underestimate or overlook significant pathways that impact human health.

When more in-depth analysis of environmental fate is required, the analyst must select the modeling procedure that is most appropriate to the circumstances. In general, the more sophisticated models are more data-, time-, and resource-intensive.

The following criteria should be considered when selecting an in-depth environmental fate model or method:

- Capability of the model to account for important transport, transformation, and transfer mechanisms;
- "Fit" of the model to site-specific and substance-specific parameters;
- Data requirements of the model, compared to availability and reliability of site information; and
- Form and content of model output. This refers to the model's ability to address important questions regarding human exposure or environmental effects and to provide all data required as input to further analysis.

Information regarding the major environmental processes that may affect the fate of hazardous substances in each medium is provided. These processes include transformation and intermedia transfer mechanisms, as well as the more complex transport mechanisms that are not incorporated into estimation procedures. By comparing the list of important processes identified for the site with the summary of model features presented at the end of each section, the analyst can select the model best suited to the requirements of the site.

The Graphical Exposure Modeling System (GEMS), developed by the EPA's Exposure Evaluation Division (EED), Office of Toxic Substances (OTS) is a set of

computer models that is easily accessible and has the ability to produce sophisticated analyses of environmental fate. GEMS consists of models capable of assessing contaminant fate in air, surface water, ground water, and soil. These fate models contain pertinent data files (including nationwide soil, land use, and meteorological data, and data on many major river systems, lakes, and reservoirs); user-input data manipulation and storage capabilities; statistical processing programs; and such graphics capabilities as presentation of results in map form.

GEMS is designed to be user-friendly. Although environmental fate modeling experience is highly desirable, personnel with no computer programming background can also use the system because of its progressive menu and user prompting formats. At each decision point, the user is presented with a list of possible selections. When specific data are required to activate a program, the system requests each type of data needed and the units required. At any point in the procedure, the user can request help from the system, and a clear explanation of the choices or steps facing the user is provided.

The GEMS host computer is a Vax-11/780, which is located at the EPA National Computer System at Research Triangle Park, North Carolina. The system can be accessed and used with the following terminal types: DEC UT-100 series, Tektronix 4014 series, and ASCII.

Terminals must be capable of transmitting or receiving ASCII data in full duplex mode, using even parity and seven-bit data word length, with communication rates of 300 or 1200 bits per second. Most common acoustic modems are compatible (GSC 1982).*

Monitoring data can also be useful in analyzing contaminant transport and fate. Monitoring results can provide, however, only a measurement of the existing extent of contamination. In addition, monitoring data alone may not allow the analyst to discriminate the contributions of specific sources to measured contaminant loadings. In all assessments, some degree of modeling contaminant movement within and among environmental media will be necessary to predict the associated exposure over a 70-year lifetime. Thus, a combination of monitoring and modeling techniques will be necessary to conduct an analysis of contaminant fate for exposure assessment purposes.

For in-depth guidance in selecting and running a computer model to use in analyzing contaminant migration from a particular site, the analyst should review the following guides:

- USEPA (1977a): Guidelines for Air Quality Maintenance Planning and Analysis, Volume 10 (Revised): Procedures for Evaluating Air Quality Impact of New Stationary Sources
- USEPA (1986b): Guideline on Air Quality Models (Revised) 1986 and Supplement A (1987)
- USEPA (1987d): Surface Water Model Selection Criteria
- USEPA (1986a): Ground Water Model Selection Criteria
- USEPA (1985j): Modeling Remedial Actions

In addition, it is recommended that the analyst obtain the user's manual for any model selected before attempting its application.

For contaminant fate in estuaries and reservoirs, the analyst should review Mills et al. (1982).

To evaluate the retardation of contaminant plumes composed of mixed wastes in ground-water systems the analyst is referred to the following references for detailed guidance: Nkedi-Kizza et al. (1985), Rao et al. (1985), Woodburn et al. (1986).

3.2 Contaminant Fate Screening

Figures 3-1 through 3-4 present the decision networks for screening contaminant fate in air, surface water, ground water, and biota. Any migration pathways (identified in the qualitative evaluation) that will require additional analysis are described in Sections 3.3 through 3.6. These pathways will be further evaluated to determine the likelihood of population exposure as described in Appendix A.

In Sections 3.2.1 through 3.2.4, brief guidance is provided for the qualitative evaluation of contaminant migration pathways. The paragraphs presented below are keyed to the accompanying decision networks and are intended to provide further elaboration of those boxes in the decision networks.

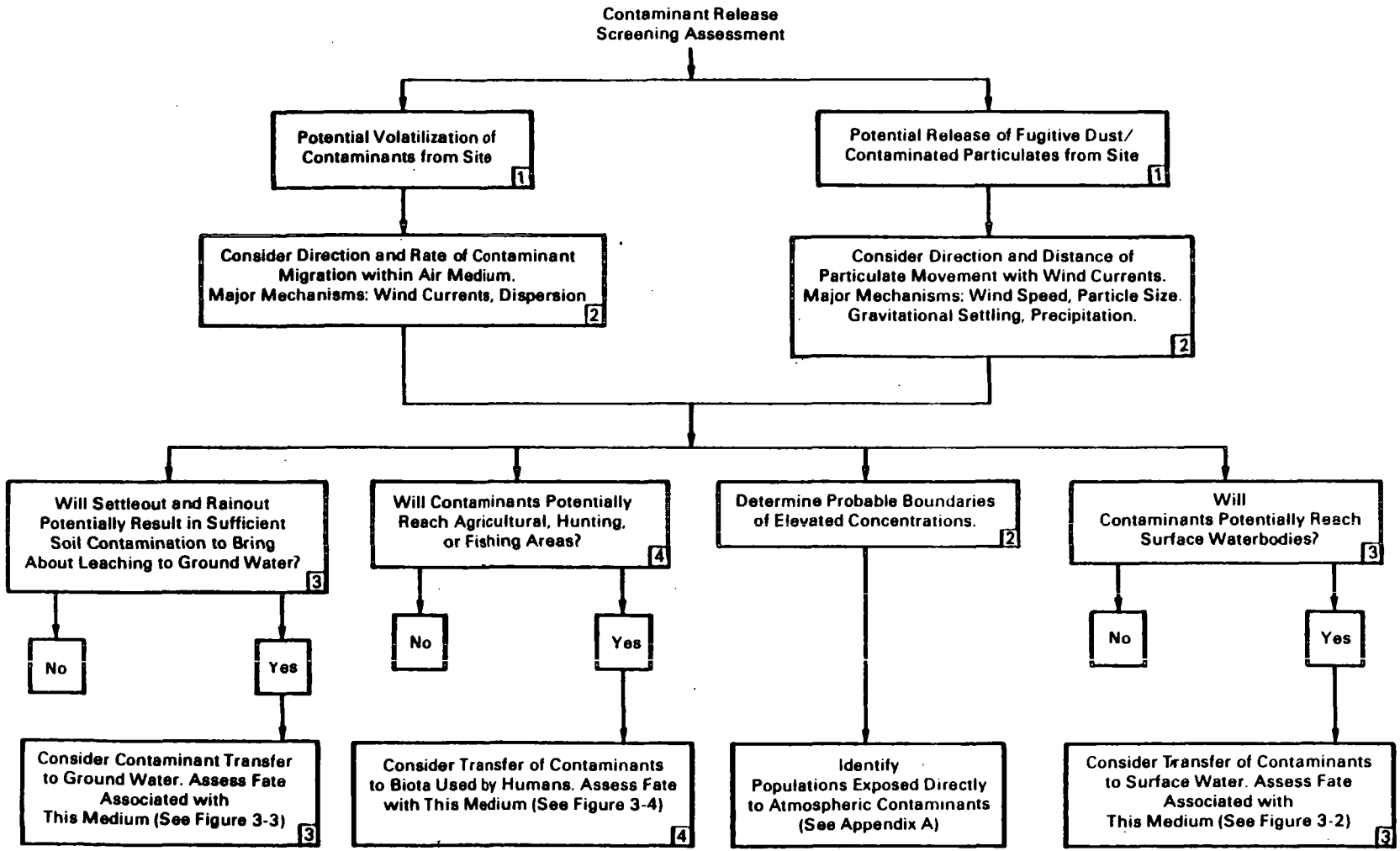
3.2.1 Atmospheric Fate

The following numbered paragraphs each refer to particular numbered boxes in the Figure 3-1.

1. The atmospheric fate of contaminants must be assessed whenever it is determined that significant

* Contact personnel within the EED are Ms. Patricia Harrigan, Mr. Loren Hall, or Mr. Russell Kinnerson. They can be reached at EPA, Washington, D.C., (202) 382-3931.

Figure 3-1. Environmental fate screening assessment decision network: atmosphere.



gaseous or airborne particulate contaminants are released from the site. The atmospheric fate of contaminants released originally to other media, but eventually partitioning to the atmosphere beyond site boundaries, must also be assessed whenever this intermedia transfer is likely to be significant.

2. The predominant directions of contaminant movement will be determined by relative directional frequencies of wind over the site (as reflected in area-specific wind rose data). Atmospheric stability and wind speeds determine off-site areas affected by ambient concentrations of gaseous contaminants. Usually, high stability and low wind speed conditions result in higher atmospheric concentrations of gaseous contaminants close to the site. High stability and moderate wind speeds result in moderate concentrations over a larger downwind area. Low stability or high wind speed conditions cause greater dispersion and dilution of contaminants, resulting in lower concentrations over larger areas.

For particulate contaminants (including those adsorbed to dust or soil particles), ambient concentrations in the atmosphere and areas affected by airborne contaminants are determined by windspeed and stability and also by particle size distribution. High winds result in greater dispersion and cause particulates to remain airborne longer (which may also increase release rates). Low winds and high stability will result in rapid settleout of particulates and in a more concentrated contaminant plume closer to the site. Larger particles will settle rapidly, decreasing the atmospheric concentrations with distance from the site. Finer particles will remain airborne longer, and their behavior will more closely approximate that of gaseous contaminants, as described above.

3. Settleout and rainout are important mechanisms of contaminant transfer from the atmospheric media to both surface soils and surface waters. Rates of contaminant transfer caused by these mechanisms are difficult to assess qualitatively; however, they increase with increasing soil adsorption coefficients, solubility (for particulate contaminants or those adsorbed to particulates), particle size, and precipitation frequency.

Areas affected by significant atmospheric concentrations of contaminants exhibiting the above physical/chemical properties should also be considered as potentially affected by contaminant rainout and settleout to surface media. Contaminants dissolved in rainwater may percolate to ground water, run off or fall directly into surface waters, and adsorb to unsaturated soils. Contaminants settling to the surface through dry deposition may dissolve in or become suspended in surface waters, or may be leached into unsaturated soils and ground water by subsequent rainfall. Dry deposition may also result in formation of a layer of relatively high contamination at the soil surface. When such intermedia transfers are likely, one should assess the fate of contaminants in the receiving media.

4. If areas identified as likely to receive significant atmospheric contaminant concentrations include areas supporting edible biota, the biouptake of contaminants must be considered as a possible environmental fate pathway. Direct biouptake from atmosphere is a potential fate mechanism for lipophilic contaminants. Biouptake from soil or water following transfer of contaminants to these media must also be considered as part of the screening assessments of these media; for example, hexachlorobenzene was found to accumulate in plants (Russell et al. 1971, Gillet 1980, Trabelka and Garten 1982).

3.2.2 Surface Water Fate

The following numbered paragraphs each refer to particular numbered boxes in the Figure 3-2.

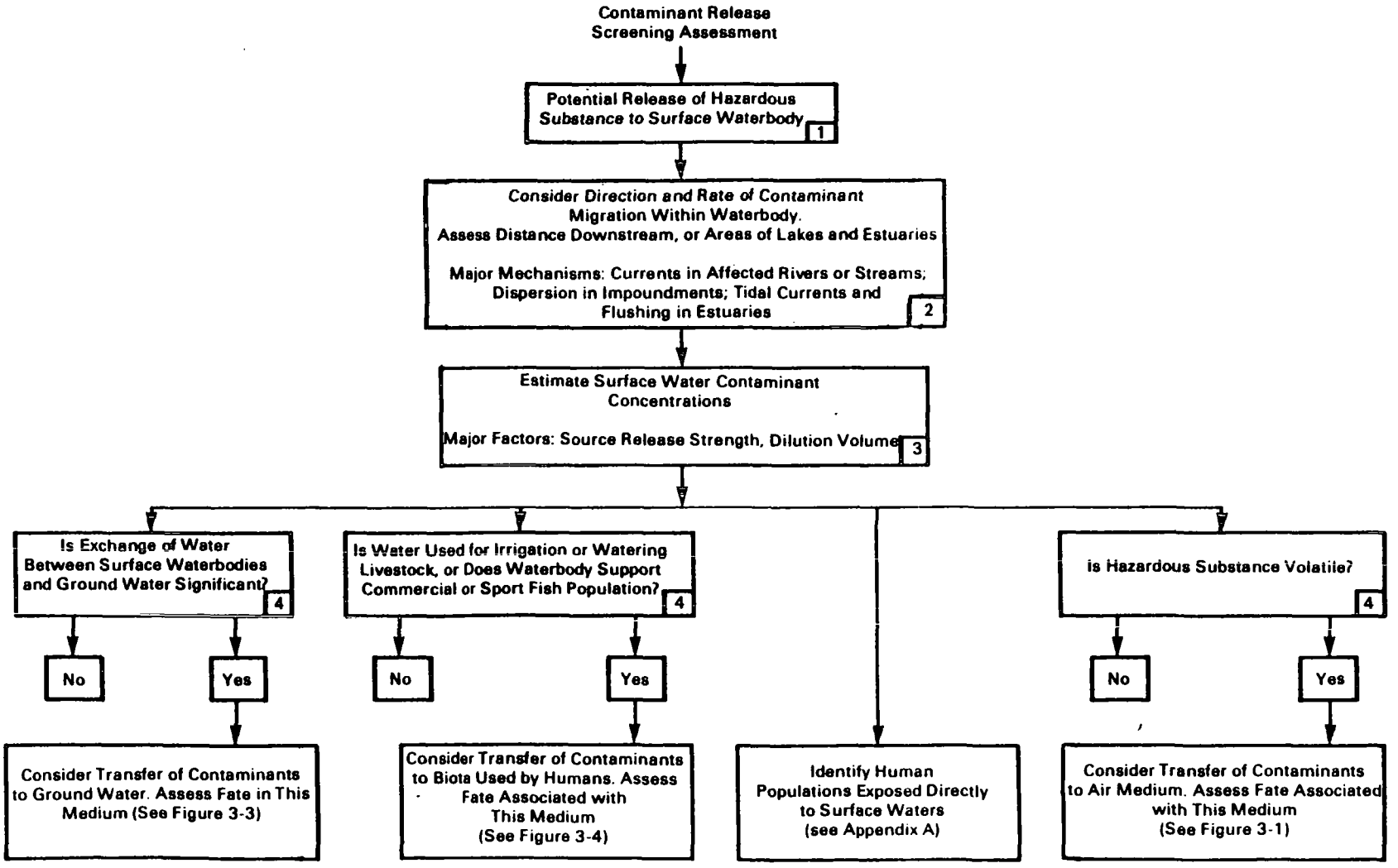
1. The aquatic fate of contaminants released from the CERCLA site as well as those transferred to surface water from other media beyond site boundaries must be considered.

2. Direction of contaminant movement will usually only be clear for contaminants introduced to rivers and streams. Currents, thermal stratification or eddies, tidal pumping, and flushing in impoundments and estuaries render qualitative screening assessment of contaminant directional transport highly conjectural for these types of waterbodies. In most cases, entire waterbodies receiving contaminants must be considered potentially significant human exposure points. More in-depth analyses or survey data may subsequently identify contaminated and unaffected regions of these waterbodies.

3. Similarly, contaminant concentrations in rivers or streams can be roughly assessed based on rate of contaminant introduction and dilution volumes. Estuary or impoundment concentration regimes are highly dependent on the transport mechanisms enumerated above. Contaminants may be localized and remain concentrated, or disperse rapidly and become diluted to insignificant levels. The conservative approach is to conduct a more in-depth assessment and use model results or survey data as a basis for determining contaminant concentration levels.

4. Important intermedia transfer mechanisms that must be considered where significant surface water contamination is expected include transfers to ground water where hydrogeology of the area indicates significant surface-water/ground-water exchange; transfers to biota where waters contaminated with

Figure 3-2. Environmental fate screening assessment decision network: surface water.



lipophilic substances support edible biotic species; and transfer to the atmosphere where surface water is contaminated by volatile substances. High temperatures, high surface-area-to-volume ratios, high wind conditions, or turbulent stream flow also enhance volatilization rates.

Contaminant transfer to bed sediments represents another significant transfer mechanism, especially in cases where contaminants are in the form of suspended solids, or are dissolved. hydrophobic substances that can become adsorbed by organic matter in bed sediments. For the purposes of this manual, sediments and water are considered part of a single system because of their complex interassociation. Surface water/bed sediment transfer is reversible; bed sediments often act as temporary repositories for contaminants and gradually re-release contaminants to surface waters. Sorbed or settled contaminants are frequently transported with bed sediment migration or flow. Transfer of sorbed contaminants to bottom-dwelling, edible biota represents a fate pathway potentially resulting in human exposure. Where this transfer mechanism appears likely, the biotic fate of contaminants should be assessed.

3.2.3 Soil and Ground-water Fate

The following numbered paragraphs each refer to particular numbered boxes in Figure 3-3.

1. The fate of contaminants in the soil medium is assessed whenever the contaminant release atmospheric or fate screening assessments results show that significant contamination of soils is likely.

2. The most significant contaminant movement in soils is a function of liquid movement. Dry, soluble contaminants dissolved in precipitation, run-on, or human-applied water will migrate through percolation into the soil. Migration rates are a function of net water recharge rates and contaminant solubility.

Liquid contaminants may percolate directly into soils. Organic liquids may alter soil permeabilities or may be of lower viscosity and/or higher density than water, resulting in percolation rates many times greater than that of water. Contaminants with high soil adsorption coefficients may bind to soils and become relatively immobile.

3. Important intermedia transfer mechanisms affecting soil contaminants include volatilization or resuspension to the atmosphere and biouptake by plants and soil organisms. These, in turn, introduce contaminants to the food chain.

4. The fate of contaminants in ground water is assessed whenever site contaminant release screening analysis indicates direct introduction of contaminants to ground water (e.g., through disposal wells or fluid releases to an aquifer near the ground surface), or whenever the screening assessments of atmospheric, surface water, or soil contaminant fates (as outlined above) indicate potential contaminant transfer to ground water.

5. The qualitative assessment of ground-water flow is often based on the assumption that subsurface hydrologic gradients (which determine flow directions and rates) approximate surface topography. This approach is unreliable and should be used only in the absence of hydrogeologic data. Ground-water flow is influenced by many factors including hydraulic conductivity of soils, hydraulic gradient, presence of subsurface impermeable barriers, presence of discharge areas (e.g., streams intercepting ground-water flow) and presence of fissures, cavities, or macropores. Hydrogeologic survey data (where available) provide a more reliable basis for contaminant transport assessment than do surface topographs.

6. Site and surrounding community survey data describing the location of wells are compared with the expected subsurface contaminant plume boundaries to identify locations of potential exposure points.

7. Important mechanisms of contaminant transfer from ground water to other environmental media include contaminated water exchange between surface waters and ground water and uptake of contaminants by edible biota. The former mechanism must be considered whenever surface waters are downgradient from the CERCLA site; it increases in likelihood with closer proximity of these surface waters to the site. Available hydrogeologic information for the site and surroundings should be reviewed for any indication that the aquifer underlying the site is connected to surface waters.

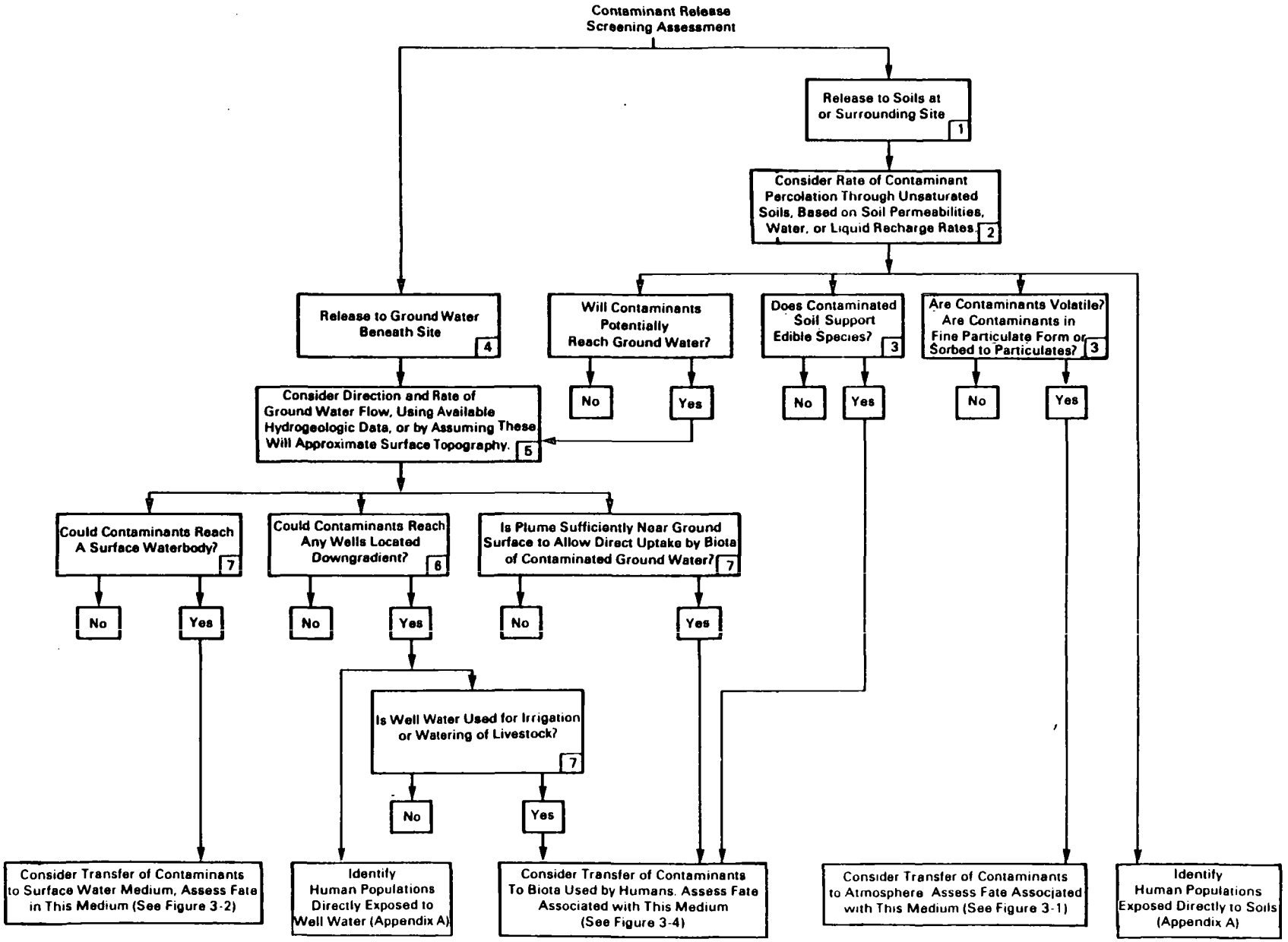
The second major intermedia transfer mechanism, biouptake, may occur through two pathways: (1) direct exposure of plants and lower trophic level animals to contaminated ground water in regions where the ground-water level is close to or at the soil surface (e.g., marshy areas, areas adjacent to aquifer discharge points), and (2) biotic exposure to ground water resulting from human activities such as irrigation or watering of livestock with well water.

3.2.4 Biotic Fate

The following numbered paragraphs each refer to particular numbered boxes in Figure 3-4.

1. A screening environmental fate assessment for the biotic medium is performed after the fate of contaminants in the atmosphere, surface waters, or ground water has been assessed. Starting with the expected distribution of contaminants in each of these media, potential points of biotic contact with

Figure 3-3. Environmental fate screening assessment decision network: soils and groundwater



contaminated media and important affected biotic species are identified.

2. Important species are those used directly by man (game animals, sport or commercial fish, crustaceans and mollusks, agricultural crops and livestock; naturally-occurring fruits, herbs, other edible vegetation), and those that introduce contaminants to species used by man through the food chain (e.g., livestock feed crops; or plants and lower trophic-level animals consumed by any of the animal groups listed above).

3. Assessed mechanisms of transport in the biotic medium include the food chain, natural animal migration, or human commercial activity. Food chain transport can result in high concentrations of contaminants in the tissue of edible species not in direct contact with contaminated air or water. Human commercial transport and natural migratory behavior of contaminated species can result in a wide distribution of edible species or tissue-containing contaminants.

4. Edible tissue concentrations are a function of the level and type of biotic exposure to contaminants, the partitioning of contaminants between organic tissue and substrate media, the biodegradability of contaminants, organism-specific metabolic characteristics, and ecosystem characteristics.

3.3 Quantitative Analysis of Atmospheric Fate

3.3.1 Screening Analysis

The atmospheric fate of substances released from uncontrolled hazardous waste sites can be estimated by using the following equation to estimate ground-level atmospheric concentrations of pollutants at selected points on a centerline of a plume directly downwind from a ground-level source (Turner 1970):

$$C(X) = \frac{Q}{\pi \sigma_y \sigma_z \mu} \qquad (3\text{-}1)$$

where

$C(X)$	=	concentration of substance at distance x from site, (mass/volume).
Q	=	release rate of substance from site, (mass/time).
σ_y	=	dispersion coefficient in the lateral (crosswind) direction, (distance).
σ_z	=	dispersion coefficient in the vertical direction, (distance).
μ	=	mean wind speed, (distance/time).
π	=	the value pi = 3.14.

The appropriate dispersion coefficients can be obtained from Figures 3-5 and 3-6. These figures provide values for σ_y and σ_z, respectively, as functions of downwind distance, x, and stability classes A though F. These stability classes are based on the Pasquill stability classification system, where Class A is very unstable and Class F is moderately stable (Pasquill 1961). Table 3-1 presents a brief illustration of how stability classes are defined.

Figure 3-4. Environmental fate screening assessment decision network: food chain.

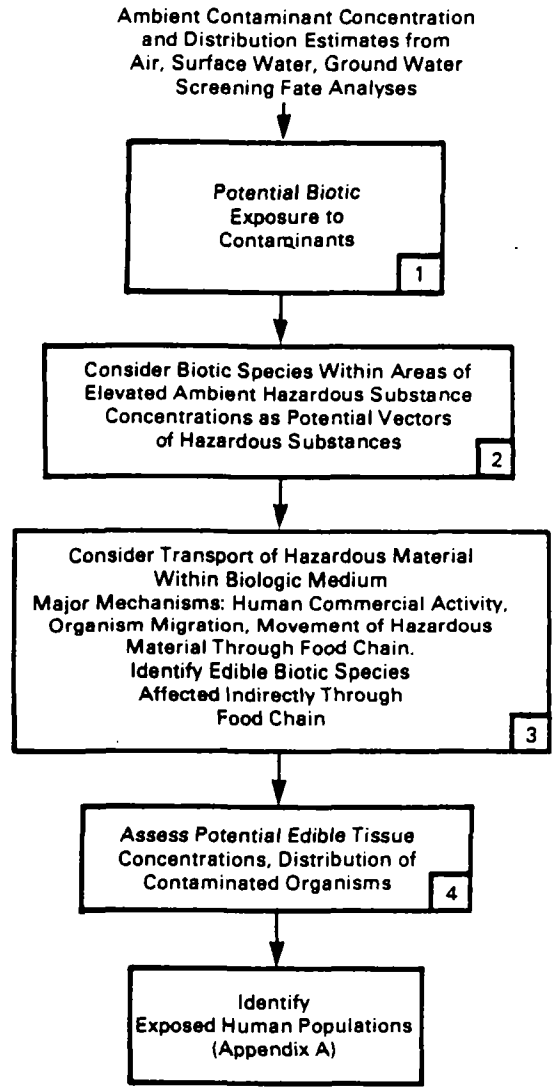
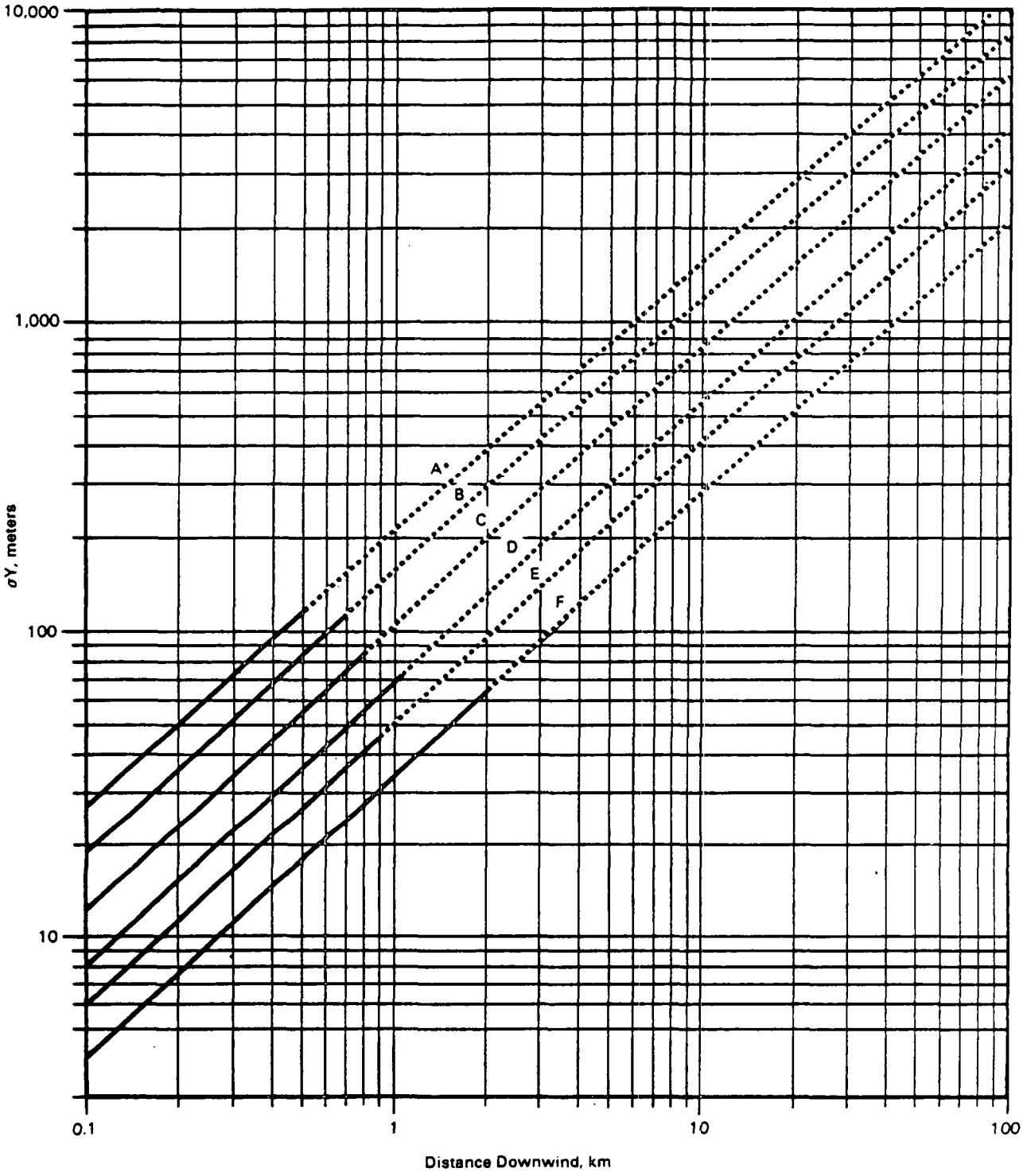
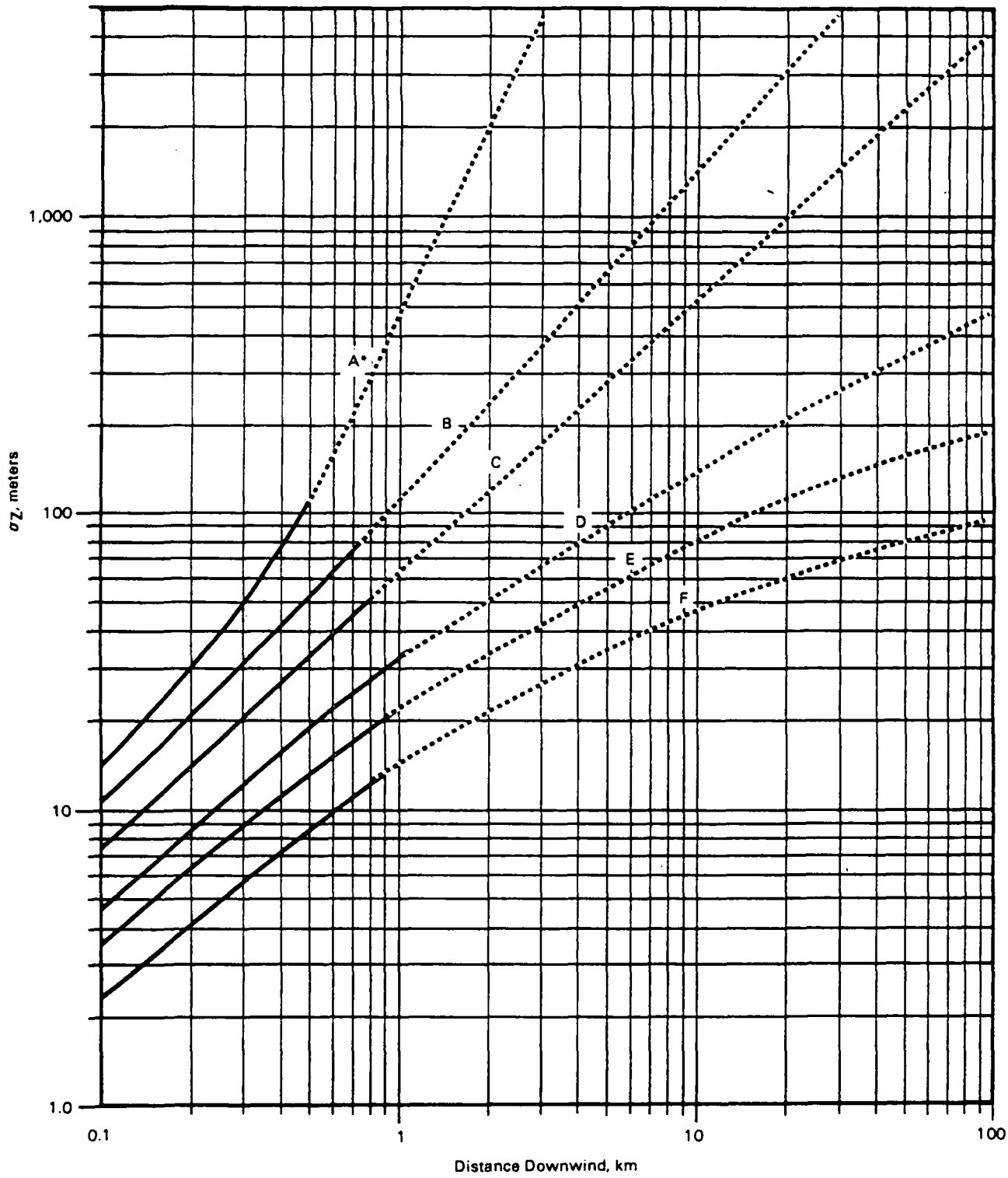


Figure 3-5. Horizontal dispersion coefficient as a function of downwind distance from the source (from Turner 1970).



*Lines designated A through F represent dispersion coefficient functions for atmospheric stability classes A through F. See text for sources of atmospheric stability data.

Figure 3-6. Vertical dispersion coefficient as a function of downwind distance from the source (from Turner 1970).



*Curves designated A through F represent dispersion coefficient functions for atmospheric stability classes A through F. See text for sources of atmospheric stability data.

Table 3-1. Key to Stability Categories

Surface wind speed at a Height of 10 m (m/sec)	Day incoming solar radiation (insolation)*			Night	
	Strong	Moderate	Slight	Thinly overcast or ≥4/8 Low Cloud Cover	≤ 3/8 Cloud Cover
<2	A	A-B	B		
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

The neutral class (D) should be assumed for all overcast conditions during day or night.
*Appropriate insolation categories may be determined through the use of sky cover and solar elevation information as follows:

Sky cover	Solar elevation angle > 60°	Solar elevation angle ≤ 60° but > 35°	Solar elevation angle ≤ 35° but > 15°
4/8 or Less or Any Amount of High Thin Clouds	Strong	Moderate	Slight
5/8 to 7/8 Middle Clouds (7000 feet to 16,000 foot base)	Moderate	Slight	Slight
5/8 to 7/8 Low Clouds (less than 7000 foot base)	Slight	Slight	Slight

Source: USEPA 1977b

To obtain the maximum hourly concentration, select the calculational methodology for coning and fanning plumes in USEPA (1977b). To obtain the estimated maximum concentration for a 3-, 8-, or 24-hour averaging time, multiply the 1-hour maximum by the factors given in USEPA (1977b).

To estimate long-term mean atmospheric concentrations, obtain STAR (Stability Array) data specific to the site. These data provide seasonal or annual joint frequencies for each stability class, wind direction, and wind speed category. Assume an annual average wind speed of 3 meters/second, and calculate the long-term mean atmospheric concentration for each exposed population by applying a weighted average, based on the relative frequency of each stability class and of wind flow toward selected exposure points. Equation 3-2 provides a rough weighted average estimate (Turner 1970):

$$\bar{C}(x) = W(x)\,[C_A(x)f_A + C_B(x)f_B + C_C(x)f_C + C_D(x)f_D + C_E(x)f_E + C_F(x)f_F] \qquad (3\text{-}2)$$

where

$\bar{C}(x)$ = average concentration at point x over long term.

$W(x)$ = relative annual frequency of wind flow towards point x.

$C_A(x)$ = concentration at point x during stability class A (from Equation 3-1).

f_A = relative annual frequency of stability class A for the specified wind direction.

and subscripts B through F represent the various stability classes.

Note that this estimate is a rough approximation because it is simplified by the assumption that the mean wind speed is 3 meters/second for all stability classes. A more sophisticated estimate can be made by incorporating site-specific wind speed frequency data, and performing similar weighted average calculation of ambient concentrations. This is a time-consuming procedure, however, and the use of computer-based estimation procedures may be more cost-effective if sophisticated estimates are required. STAR data are available from the National Climatic Center (NCC), Asheville, North Carolina (phone: (704) 259-0205) for all National Weather Service (NWS) locations in the U.S. The NWS Station that is most representative of the site should be used.

The area within which the ground-level concentration of a hazardous substance is above a predetermined critical concentration (i.e., the plume isopleth) can be described using the following procedures. Calculate the crosswind distance from any point along the plume centerline (i.e., perpendicular to the plume centerline) to the isopleth boundary by Equation 3-3 (Turner 1970):

$$y_{(X)} = 2\ln\left(\frac{C(x)}{C(CL)}\right)^{1/2}\left(\sigma_y\right) \qquad (3\text{-}3)$$

where

$C(CL)$ = predetermined critical concen-tration level, (mass/volume).

$y_{(x)}$ = perpendicular distance from point on plume centerline to the C(CL) isopleth boundary, (length units).

$C(x)$ = concentration at plume centerline, x distance from source, (mass/volume, as calculated by Equation 3-1).

σ_y = lateral dispersion coefficient, (length units).

Vary the value for x (downwind distance from the source) input into Equations 3-1 and 3-3, starting at a point near the site* and increasing this value until the value for C(x) (obtained from Equation 3-1) equals the predetermined critical concentration C(CL). Values calculated for y describe the isopleth boundary on either side of the plume centerline.

* Equations are generally considered applicable to downwind distances of at least 200 m.

Estimate the area within a plume isopleth using Figure 3-7 which plots the value $C(CL)\mu$ (relative concentration times wind speed versus isopleth area, for each stability class A through F).

All of the preceding simplified equations provide atmospheric fate estimates based on several simple assumptions, one of which requires special mention. This is the assumption that the hazardous substance released from a site is in a form that can remain airborne indefinitely (i.e., either gaseous or consisting of particles less than 20 microns in diameter) (Turner 1970).

In cases where fugitive dust blown from the site includes solid hazardous substances (or soil particulates carrying adsorbed hazardous substance) of greater diameter than 20 microns, relatively rapid gravitational settling of the larger particles occurs. Consequently, much of the hazardous material reaches the ground before advection and dispersion can transport and dilute the plume as described by the above equations. Thus, areas close to the uncontrolled hazardous site may experience significant soil contamination, and human exposure points farther from the site may experience lower atmospheric concentrations than estimated by these equations. Hanna and Hosker (1980) present a procedure for estimating the gravitational settling rate, distance of travel from the source, and deposition rate of airborne particulates.

All of the above simplified procedures incorporate the following additional assumptions:

- Steady-state condition, i.e., windspeed is steady at rate u, and the hazardous substance release is continuous, at average rate Q. Wind direction is also assumed to be steady; short-term fluctuations are disregarded.
- Longitudinal dispersion is negligible (substance travels at wind speed in the downwind direction).
- The substance is refractory (all removal and decay processes are disregarded).
- The substance is distributed normally, or according to a Gaussian distribution, both vertically and in the crosswind direction.
- The air environment is homogeneous; wind speeds and stability are equal at all heights above the ground, and no obstructions to wind flow or dispersion exist other than at the ground. Complete reflection occurs at the ground/air interface.

3.3.2 In-Depth Analysis

Where estimates of ambient atmospheric concentrations of hazardous substances developed by the preceding simplified procedures indicate that these concentrations pose potential health hazards, more accurate, in-depth analysis of atmospheric fate may be required. Numerous computer models are available for this purpose and are listed in USEPA (1986b). These models vary in sophistication and capability, and in their ability to incorporate expressions describing the effect of various processes on the atmospheric fate of hazardous substances. The most important of these processes are briefly described below. Consider the importance of each of these processes to the atmospheric fate of the substances under analysis before selecting a computer model.

3.3.2.1 Intermedia Transfer

The following are the most important processes that affect the removal of hazardous substances from the air medium and their transfer to other sectors of the environment.

(1) Dissolution

This is the process whereby hazardous substances in the gaseous state are dissolved into water droplets present in the atmosphere. This process, followed by precipitation, distributes the substance over the surface media, and percolation to ground water may follow. Direct dissolution may also occur between gaseous substances in the atmosphere and surface waters at the air/water interface. Dissolution is a constant, reversible process, the amount of hazardous substance in the aqueous phase is determined by the partition coefficient of the substance between the gas and aqueous phases. This partition coefficient is in turn a function of the vapor pressure and water solubility of the substance, its concentration in the air, and temperature. See Lyman et al. (1982) or Hanna and Hosker (1980) for methods of estimating this partition coefficient and atmospheric half-lives resulting from dissolution/ rainout.

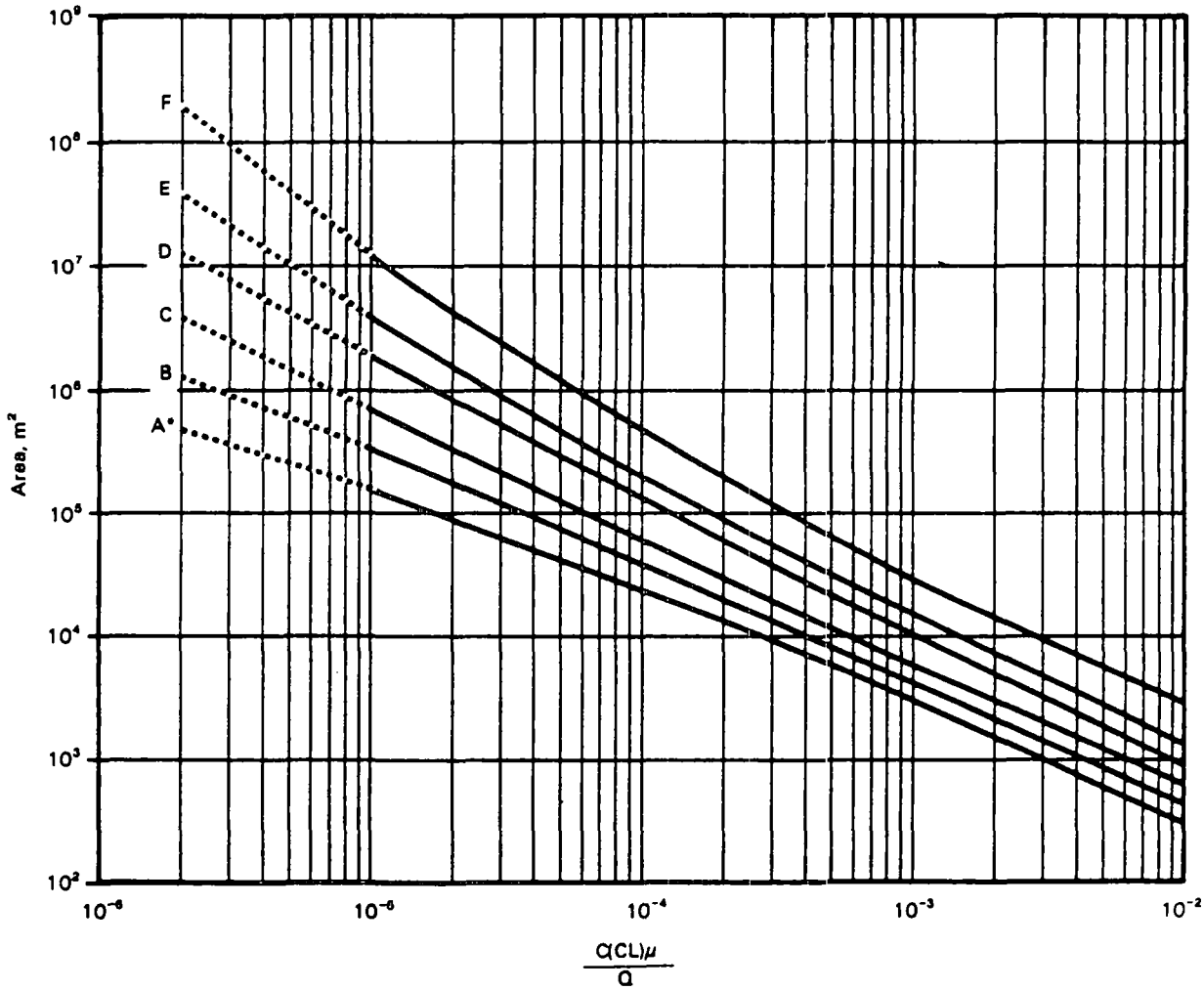
(2) Adsorption

Through the process of adsorption, hazardous substances in the vapor phase become attached to particulate matter suspended in the air (aerosols), or onto soil particles at the air/soil media interface. Suspended aerosols settle to surface media, thereby removing adsorbed substances from the air environment. The adsorption rate of a particular substance is principally a function of the number and surface area of aerosols per volume of air, the molecular weight of the substance in question, its concentration in the air, and its saturation vapor pressure. Cupitt (1980) provides a method for estimating atmospheric contaminant removal rates due to adsorption to particulates and settleout.

(3) Gravitational Settling

This mechanism is most important for particulate hazardous substances, or hazardous substances

Figure 3-7. Area within isopleths for a ground-level source (Hilsmeir and Gifford 1962, as presented by Turner, 1970).



*Curves designated A through F represent functions for atmospheric stability classes A through F. See text for sources of atmospheric stability data.

adsorbed onto suspended particulates, if the particulate matter is more than 20 μm in diameter. These particles settle to the surface media at a rate that is a function of their density, shape, and diameter, and of wind speed (Hanna and Hosker 1980).

(4) Precipitation

Precipitation itself is a major mechanism for removal of particulate and aerosol matter. Raindrops require particulates or aerosols to serve as nuclei for their condensation from the vapor state of water. Moreover, raindrops generally remove particulates and aerosols >1.0 μm in diameter as they fall below the cloud level.

3.3.2.2 Intramedia Transformation Processes

Many hazardous substances are subject to decay or transformation to other substances with new properties while entrained in the air environment. The two most important of these processes are described below. While the product of such transformation processes will usually have different properties from those of the original hazardous substance, the new substance produced may also have hazardous properties. Cupitt (1980) provides estimates of

constants that determine the rate of each transformation process below, as well as of the importance and likely products of these processes, for 46 hazardous materials. Hendry and Kenley (1979) provide rate constants and estimation procedures for these processes.

(1) Photolysis
This is the breakdown of substances because of photochemical reaction brought about by solar energy. Photolysis can be direct, when the hazardous substance is itself affected by solar radiation, or indirect when the hazardous substance reacts with other substances that have been raised to a reactive state by solar radiation. Photolysis rates depend on solar radiation availability, the light absorption coefficient of the hazardous substances, and a reaction yield constant (which describes the efficiency of transformation of the hazardous substance with the available sun energy).

(2) Oxidation
The reaction of substances with oxidants in the atmosphere can result in their transformation. The two most important atmospheric oxidants are ozone and the hydroxyl radical. Reaction rate constants for oxidation are chemical specific; the overall rate of transformation of a hazardous substance by oxidation depends on the concentration of the oxidant and the reaction rate constant.

3.3.2.3 The Effects of Terrain
Features such as vegetation, large buildings, urban areas, rough topography, hills, or mountains can all profoundly affect the atmospheric fate of airborne substances, principally by altering the laminar flow of transporting wind currents. The effects of terrain on wind currents may include increased turbulence, downwash in the lee of large obstacles, or localized alterations in the direction of flow. Because the release of substances from hazardous waste sites usually occurs at ground level, the fate of these substances is especially susceptible to the effects of terrain. Select a model capable of accounting for these effects in any case where these listed terrain features exist between the site and points of human exposure.

3.3.3 Computer Models
Tables 3-2, 3-3, and 3-4 provide general information about computer-based models that could be appropriate to in-depth analysis of the atmospheric fate of substances released from CERCLA sites. Table 3-2 contains resource requirements, references, and sources for each model; Table 3-3 summarizes their features and capabilities; and Table 3-4 discusses the data requirements of each. By comparing the information in these tables with identified site features, site data availability, final output requirements, and resource availability, one can select the most applicable and cost-effective model.

The Industrial Source Complex (ISC) long-term model and the TOXBOX area source model are presently integrated into the GEMS system. These models are accessed under a subsystem of GEMS referred to as the GEMS Atmospheric Modeling System (GAMS). A brief description of ISC is provided below.

The ISC (Bowers et al., 1979) is a Gaussian dispersion model, capable of estimating the concentration and deposition rates of gaseous and particulate pollutants around a point, area, or line source. Because it is integrated into the GEMS system, it is especially useful for the analysis of the atmospheric fate of hazardous substances. Based on a user-input release location (in the form of latitude/longitude coordinates or zip code), stored climatological data from the nearest meteorological monitoring stations are retrieved (GSC 1982).

The integration of ISC with a population distribution model called SECPOP gives it the capability of expressing atmospheric fate of pollutants in terms of numbers of people affected at various concentration levels (this capability is discussed in more detail in Appendix A, Exposed Populations).

The ISC model can estimate the concentration of pollutants released from point, area, or line sources. Area sources are simulated by use of a virtual point, and line sources by a series of points. Short-term (hourly) or long-term (seasonal, annual average) concentration estimates can be developed, and gravitational settling can be simulated based on user-input half-life data (GSC 1982).

ISC can be used with IBM, CDC, or VAX computers. The model is implemented within GEMS on EPA's VAX 11/780 and can be accessed with a variety of user terminal types. (See Section 3.1 for access instructions.)

3.3.4 Short- and Long-Term Concentration Calculations
Long-term average ambient air concentrations of hazardous substances at human exposure points are estimated using the long-term average release rate over the time period of interest, and the weighted averaging algorithm presented as Equations 3-1 and 3-2. Annual average climatological data, or STAR data including long-term frequencies of all climatological parameters, should be used as input to these equations.

Where site-specific data are unavailable, short-term concentration levels are estimated using the maximum short-term release rate and climatological assumptions presented in Table 3-1. When using

Table 3-2. Resource Requirements and Information Sources: Atmospheric Fate Models

Model	Description	Resource Requirements, comments	References, sources of documentation, software
Box Model	• Area Source. • Vertical dispersion or no vertical dispersion option. • Basic box model.	• Available through GEMS (see Section 3.1).	
Climatological Dispersion Model (CDM)	• Long-term seasonal or annual. • Point or area sources. • Gaussian plume model. • Simulates nonconservative pollutants. • Can simulate turbulence over urban areas. • Outputs long-term average concentrations at user-specified receptors.	• Requires stability array data. • FORTRAN V program language; has been implemented on the UNIVAC 1110. • 22 K bytes storage required. • Software available as part of UNAMAP package for $420.	*Documentation:* Busse and Zimmerman 1976 *Software*: Computer Products, NTIS, Springfield, VA. 22161
Industrial Source Complex	• Operates in both long-term and short-term modes. • Accounts for settling and dry deposition of particles; downwash, area, line, and volume sources; plume rise as a function of downwind distance; separation of point sources; and limited terrain adjustments. • Appropriate for industrial source complexes, rural or urban areas, flat or rolling terrain, transport distances less than 50 kilometers, and one hour to annual averaging times.	• Integrated into GEMS (see Section 3.1). • Source data: location, emission rate, physical stack height, stack gas exit velocity, stack inside diameter, and stack gas temperature. Optional inputs include source elevation, building dimensions, particle size, distribution with corresponding settling velocities, and surface reflection. • Meteorological data: includes stability wind rose (STAR deck), average afternoon mixing height, average morning mixing height, and average air temperature.	*Documentation:* Bowers et al. 1979 *Software*: Computer Products, NTIS, Springfield, VA. 22161
Ram	• Steady-state Gaussian plume model. • Appropriate for point and area sources, urban areas, flat terrain transport distances less than 50 kilometers, and one hour to one year averaging times. • May be used to model primary, pollutants, however settling and deposition are not treated.	• Available code on UNIMAP (Version 6). • Source data: point sources require location, emission rate, physical stack height, stack gas exit velocity, stack inside diameter and stack gas temperature. Area sources require location, size, emission rate, and height of emission. • Meteorological data: hourly surface weather data from the preprocessor RAMMET. Actual anemometer height is also required.	*Reference*: Turner and Novak, 1978.
CRSTER	• Steady-state Gaussian dispersion model. • Designed to calculate concentrations from point sources at a single location. • Highest and high-second high concentrations are calculated at each receptor. • Appropriate for single point sources, rural or urban areas, transport distances less than 50 kilometers, and flat or rolling terrain.	• Available on UNIMAP (Version 6). • Source data. emission rate , physical stack height, stack exit velocity, stack inside diameter and stack gas temperature. • Meteorological data: hourly surface weather data from the preprocessor RAMMET. Actual anemometer height is also required.	*Reference*: USEPA 1977b.

(Continued)

Table 3-2. (Continued)

Model	Description	Resource Requirements , comments	References, sources of documentation, software
Texas Climatological Model Control (TCM)*	• Long-term (seasonal or annual). • Gaussian dispersion. • Two pollutants per run. • Includes option for simulation of urban area turbulence classes. • Handles nonconservative pollutants. • Point or area sources. • Up to 2,500 receptor locations on downwind user-specific grid. • Outputs average concentration data.	• Requires stability array data. • FORTRAN program language; has been implemented on Burroughs 6810/11. • Batch mode. • 17 K bytes memory required. • Technical background in meteorology, air pollution useful.	*Documentation*: Texas Air Control Board 1980.
Texas Episodic Model (TEM)*	• Steady-state model. • Point or area sources. • Short-term - 10 minutes to 24 hours. • Produces maximum and average concentrations over time periods selected by user. • User can select up to 2,500 downwind receptor points, according to an automatic or specified grid array. • Handles nonconservative pollutants. • Up to 24 meteorologic scenarios can be input for a single run.	• FORTRAN program applicable to a wide range of computer types; has been implemented on Burroughs 6810/11. • Requires approximately 26 K bytes memory. • Engineering, meteorology, atmospheric transport background useful.	*Reference*: Christiansen 1976.
Model MPTER	• Multiple point source algorithm useful for estimating air quality concentration of relatively non-reactive pollutants. • Appropriate for point sources, rural or urban areas, flat or rolling terrain, transport distances less than 50 kilometers, and one hour to one year averaging times.	• Source data: location, emission rate , physical stack height, stack gas exit velocity, stack inside diameter, stack gas temperature, and optional ground level elevation. • Meteorological data: hourly surface weather data from the preprocessor RAMMET. Actual anemometer height is also required.	*Documentation*: Pierce and Turner 1980. Chico and Catalano 1986.
VALLEY**	• Short- or long-term. • Simulates plume impact in complex terrain. • Provides screening estimates of worst-case short-term concentrations. • Provides annual average concentrations. • 12-receptor grid.	• May require careful analysis of output by experienced air quality modeler. • FORTRAN V program, applicable to wide range of computers. • Approximately 13 K bytes memory required.	*Reference*: Burt 1977. Software: Computer Products, NTIS, Springfield, VA 22161.

Sources: Bonazountas et al. 1982; USEPA 1979; USEPA 1982a.
*These models are not EPA preferred models. They can, however, be used if it can be demonstrated that they estimate concentrations equivalent to those provided by the preferred models, e.g., CDM, RAM, ISC, MPTER, CRSTER, for a given application.
**This model is recommended for screening applications only.

Table 3-3. Features of Atmospheric Fate Models

	HANDLES PARTICULATE RELEASES	HANDLES VOLATILIZATION RELEASES	POINT SOURCE	AREA SOURCE	MULTIPLE SOURCE	ACCOUNTS FOR HORIZONTAL DISPERSION	ACCOUNTS FOR VERTICAL DISPERSION	ACCOUNTS FOR DEGRADATION	ACCOUNTS FOR DISSOLUTION/RAINOUT	HANDLES ROUGH TERRAIN/URBAN SIMULATION	ACCEPTS TIME-VARIANT RELEASE TERMS	PRODUCES 24-HOUR MAXIMUM AMBIENT CONCENTRATION DATA	PRODUCES ANNUAL AVERAGE CONCENTRATION DATA (FOR PARTICULATE RELEASES)	PRODUCES RATE OF DEPOSITION FOOTPRINTS	OUTPUT IN FORM OF ISOPLETHS OR DATA SUFFICIENT FOR ISOPLETH CHARTING	OUTPUT IN FORM OF CONCENTRATIONS AT RECEPTOR POINTS
TEM		●	⊖	⊖	⊖	⊖	⊖	⊖					⊖	⊖		⊖	⊖
TCM *		●	●	●	●	●	●	●			●			●		●	●
CDM		●	●	●		●	●	●	●	●				●		●	●
VALLEY **		⊖	⊖	⊖	⊖	⊖	⊖	⊖	⊖	⊖			⊖	⊖			
ISC	⊖	⊖	⊖	⊖	⊖	⊖	⊖	⊖		⊖		⊖	⊖	⊖	●	⊖	⊖
BOXMOD	⊖	⊖		⊖			⊖	⊖	⊖	⊖				⊖			⊖
RAM	⊖	⊖	⊖	⊖	⊖	⊖	⊖	⊖				⊖	⊖	⊖		⊖	⊖
CRSTER	●	●	●			●	●	●			●		●	●		●	●
MPTER	●	●	●		●	●	●	●				●	●	●		●	●

Source: Bonazountas et al. 1982; USEPA 1979; USEPA 1982a.

* This model is recommended for screening applications only.

** These models are not EPA preferred models. These models can be used if they can be demonstrated to estimate concentrations equivalent to those provided by the preferred models, e.g., CPM, RAM, ISC, MPTER, CRSTER, for a given application.

Table 3-4. Data Requirements for Atmospheric Models

	SITE LOCATION (USES STORED CLIMATOLOGICAL DATA)	WIND ROSE (OR WIND SPEED FREQUENCIES IN SINGLE DIRECTION)	STABILITY ARRAY (STAR) DATA	PRECIPITATION	AMBIENT TEMPERATURE	WORST-CASE CLIMATOLOGICAL DATA ASSUMPTIONS	RECEPTOR ELEVATIONS	RECEPTOR LOCATION GRID OR POINT	TOPOGRAPHIC/VEGETATIVE COVER/ URBAN BUILDING FEATURES	EMISSION STATE (GASEOUS/PARTICULATE)	PARTICLE SIZE AND DENSITY	POLLUTANT MOLECULAR WEIGHT	ATMOSPHERIC HALF-LIFE (OVERALL DECAY) COEFFICIENT	EMISSION RATE (EXPRESSED AS STEADY STATE)	TIME-VARIANT EMISSION RATE	SOURCE DESCRIPTION (POINT OR AREA SIZE)
TEM*		●			●			●					●	●		●
TCM*		●			●			●	●				●	●		●
CDM		●	●					●	●					●		●
VALLEY**		●	●			●	●	●	●					●		
ISC		●	●							●	●				●	●
BOXMOD	●			●						●		●	●	●		●
RAM		●						●		●			●	●	●	●
CRSTER		●					●	●		●			●	●		●
MPTER		●			●		●	●		●			●		●	

Source: Bonazountas et al. 1982; USEPA 1979; USEPA 1982a.

* This model is recommended for screening applications only.

** These models are not EPA preferred models. These models can be used if they can be demonstrated to estimate concentrations equivalent to those provided by the preferred models, e.g., CPM, RAM, ISC, MPTER, CRSTER, for a given application.

site-specific data, the most stable atmospheric conditions, lowest wind speed, and greatest percent of wind flow toward the exposed population should be used as input to Equation 3-1, along with maximum release rate estimates for the duration of interest. Usually, the population nearest the point or area of a ground-level release experiences the highest short-term exposure.

As indicated in Table 3-2, several atmospheric fate models have the capability of producing short-term maximum and long-term average ambient concentration estimates where in-depth analysis is desirable.

3.4 Surface Water Fate Analysis

The environmental fate of hazardous materials entering surface waterbodies is highly dependent on the type of waterbody. The three major classifications are rivers and streams, impoundments, and estuaries. Methods for estimating contaminant concentrations in the first category are provided below.

As mentioned in the introduction to this chapter, contamination of flowing waterbodies will probably be a more common occurrence with regard to uncontrolled hazardous waste facilities than will contamination of impoundments or estuaries. Thus, in this section guidance for estimating contaminant fate in flowing waterbodies is presented. In those cases where contaminant fate in an impoundment or estuary is necessary, the analyst is referred to Mills et al. (1982) for guidance.

The Probabilistic Dilution Model is an analytical tool that can be used to extend the qualitative screening analysis presented in the previous section and that in some cases may make application of the quantitative analyses discussed in following sections unnecessary. This model has been adapted by the U.S. Environmental Protection Agency, Office of Toxic Substances, to support the exposure assessment process for contaminants in surface water. The model is based on the fact that, in general, the most important process affecting a contaminant's concentration in a surface waterbody is the degree of its dilution. Thus, the model uses streamflow data for a given subbasin and contaminant loading data (from the contaminant release analysis discussed in Chapter 2) to predict the number of times per year a given contaminant concentration will be exceeded. For contaminants that have health-based concentration standards (or for which health-based concentration cut-off values can be calculated), the model can be used to predict the annual number of occurrences (days) that unacceptable health risks may result for persons using the affected waterbody. This model can be applied to the Superfund exposure assessment process as an extended screening tool to highlight contaminant releases to surface water that actually require detailed environmental fate (and subsequent exposed populations) analysis. Contact the USEPA Office of Toxic Substances, Exposure Evaluation Division (Pat Kennedy, (202) 382-3916) for more detailed information on accessing the Probabilistic Dilution Model.

3.4.1 Beginning Quantitative Analysis

The following equation (adapted from Delos et al. 1984) provides a rough estimate of the concentration of a substance downstream from a point source release into a flowing waterbody, after dilution of the substance by the receiving waterbody:

$$C = \frac{C_e Q_e}{Q_t} \qquad (3\text{-}4)$$

where

C	=	concentration of substance in stream, (mass/volume).
C_e	=	concentration of substance in effluent, (mass/volume).
Q_e	=	effluent flow rate, (volume/time).
Q_t	=	combined effluent and stream flow rate, (volume/time).

This equation predicts the concentration of substance in the waterbody resulting from contaminant releases from the subject site alone; it does not take into account additional sources of contamination ("background" concentrations) that may also contribute to the total level of contamination in the waterbody.

In cases where hazardous waste is introduced into a stream through intermedia transfer from air, soil, ground water, or nonpoint source, or where the release rate is known in terms of mass per unit time rather than per unit effluent volumes, in-stream concentrations can be estimated by use of the following equation:

$$C = \frac{T_r}{Q_t} \qquad (3\text{-}5)$$

where

T_r	=	intermedia transfer rate, (mass/time)
Qt	=	stream flow rate after intermedia transfer has occurred, (volume/time).

Assumptions implicit in these equations are the following:

- Mixing of the hazardous substance in the water is instantaneous and complete.

- The hazardous material is refractive (i.e., all decay or removal processes are disregarded).

- Stream flow and rate of contaminant release to the stream are constant (i.e., steady-state conditions).

The assumption of complete mixing of a hazardous substance in a flowing water body is not valid within a mixing zone downstream from the point or reach where the substance is introduced. Under certain conditions, this mixing zone can extend downstream for a considerable distance, and concentrations can be considerably higher within the mixing zone than those estimated by the foregoing dilution equations.

The length of the mixing zone is estimated by the following equation (adapted from Fischer et al. 1979, Liu 1977, Neely 1982):

$$MZ = \frac{0.4\, w^2 u}{0.6 d \sqrt{g d_n s_l}} \qquad (3\text{-}6)$$

where

MZ	=	mixing zone length, (length units).
w	=	width of waterbody, (length units).
u	=	stream velocity, (length/time).
d_n	=	stream depth, (length units).
s_l	=	slope of the stream channel, (length/length).
g	=	acceleration due to gravity, (32 ft/sec^2).

These equations provide in-stream contaminant concentrations resulting from site releases only. If total in-stream contaminant concentrations are desired, these should be estimated by adding background (i.e., upstream from the site) in-stream contaminant concentrations to those estimated by Equations 3-4 and 3-5.

If the hazardous substance is introduced into a flowing waterbody over a length of that body, rather than from a point source, assume that the mixing zone begins at the downstream end of the reach over which introduction takes place. Neely (1982) presents an estimation procedure for hazardous substance concentration at exposure points within a mixing zone that incorporates an expression for dispersion.

The dilution equations (3-4, 3-5) and the procedure presented by Neely (1982) assume that the introduced hazardous substance is conservative. Therefore, they predict an estimated stream/river concentration that remains constant from the downstream end of the mixing zone throughout the remaining length of the stream, or decreases only with further dilution resulting from additional stream flow from tributaries. This is useful as a basic model for the fate of conservative hazardous substances; for nonconservative substances, it provides a useful worst-case estimate. If the released substance is found through this estimation procedure to be diluted to concentrations below a predetermined level of concern, and no important exposure points exist within the mixing zone, the fate of the substance in this medium may need no further analysis. However, where the concentration after dilution of a nonconservative substance is still above a predetermined critical level, it may be useful to estimate the distance downstream where the concentration will remain above this level, as well as the concentration of the substance at selected exposure points downstream.

This type of estimation can be performed through use of an overall decay coefficient, which represents a combination of all decay and loss rates affecting the removal of a substance from a waterbody. The concentration of a nonconservative substance at a selected point downstream from the release point and below the mixing zone (complete mixing is assumed) can be estimated by the following equation (from Delos et al. 1984), which employs the concept of an overall decay coefficient:

$$W(x) = W(O) e^{-K \frac{x}{u}} \qquad (3\text{-}7)$$

where

W(x)	=	concentration at downstream distance x, (mass/volume).
W(O)	=	concentration immediately below point of introduction, (from Equations 3-4, 3-5).
e	=	2.71828.
K	=	overall decay coefficient, (time)$^{-1}$.
x	=	distance downstream from point of introduction, (length).
u	=	stream velocity, (length/time).

The overall decay coefficient can also be used to estimate the distance downstream over which a nonconservative substance remains above a predetermined critical concentration level W(CL). This is estimated by substituting W(CL) for W(x) in Equation 3-7, and solving this equation for x, as follows:

$$x = -\frac{u}{K} \ell n\left(\frac{W(CL)}{W(O)}\right) \qquad (3\text{-}8)$$

where

x	=	distance downstream from point of introduction, (length).
u	=	stream velocity, (length/time).
K	=	overall decay coefficient, (time)-1.
W(CL)	=	predetermined critical concentration level, (mass/volume).

W(0) = concentration immediately below point of introduction, (from dilution Equations 3-4, 3-5).

This equation incorporates the following assumptions:

- Mixing is complete.
- Conditions are steady state.
- Longitudinal dispersion is negligible; the substance transports downstream at stream velocity.
- All decay and transfer processes can be described as first-order coefficients (i.e., decay rates are a direct function of hazardous substance concentration).

Values for K can be derived empirically where monitoring data are available, or can be estimated based on decay rate constants available for many hazardous substances in the technical literature.

Concentration data from immediately below the point of substance release into a stream (after complete mixing of waste stream into the waterbody), and from at least one point downstream of the mixing zone are required for the empirical estimation of K. Note that overall decay coefficients are substance- and site-specific and can vary with climatic and hydrologic conditions. Care must be taken in calibrating the coefficient empirically. Data covering seasonal fluctuations must be used, and seasonal values for K corresponding to the various observed conditions, or a worst-case K value (i.e., lowest reasonable value) for the purpose of conservative estimation, should be developed.

For estimation of K through the summation of published decay rate constants, the most important removal process affecting the compound of concern in the receiving waterbody must be known. For this information, see the discussion below (Section 3.4.2), or see Callahan et al. (1979), or Mabey et al. (1982). Additional references that provide decay rate constant values for a wide variety of compounds include: Verschueren (1984), Dawson et al. (1980), USCG (1974), and Schnoor et al. (1987).

Reliable values for K, which have been developed for a given waterbody and hazardous substance under no-action conditions (i.e., during remedial investigation), can be used to estimate the fate of this same substance resulting from the release rates projected after implementation of various remedial action alternatives.

3.4.2 In-Depth Analysis

When aquatic concentration estimates developed by the above simplified methods (or methods covering estuaries or impoundments provided by Mills et al. 1982) indicate that these concentrations pose a potential human health hazard at one or more exposure points, more accurate estimates of short-term and long-term concentrations of the hazardous substance may be required. A large number of in-depth methods and computer models exist to assess the fate of substances in the aquatic environment. Each of these models differs in the number and types of aquatic fate processes that it incorporates. The most important of these aquatic processes are described below, and information is provided to allow identification of those processes most likely to be significant at the site, and for the hazardous substances under analysis.

3.4.2.1 Intermedia Transfers

The major processes by which hazardous substances can be transferred from surface water to other environmental media are as follows:

(1) Volatilization

Volatilization of a substance from water depends on the physicochemical properties of the substance and characteristics of the waterbody and body of air involved. Volatilization increases in importance for substances with higher vapor pressure, and for waterbodies with higher surface area-to-volume ratios and higher turbulence (Delos et al. 1984). Callahan et al. (1979) stress the importance of volatilization as a route of intermedia transfer for 129 priority pollutants. If volatilization is considered an important process for the substance being studied, or if the importance of volatilization is unknown, the rate of volatilization can be estimated by the method provided by Mills et al. (1982) for quiescent waterbodies or by Delos et al. (1984) for turbulent bodies. Lyman et al. (1982) provide methods for estimating volatilization rates from water.

(2) Sedimentation

Hazardous substances released to a surface waterbody in the solid, particulate form will settle out over time and become mixed into the bottom sediment. In addition, liquid hazardous substances with high affinities for adsorption to suspended particulates will settle out of surface waters with these particulates. The rate of sedimentation is governed by the difference between settling velocity and resuspension velocity. The former increases with mean particle size and density and with water temperature, and can be estimated by the procedure presented by Delos et al. (1984). Resuspension velocity is a function of bottom shear stress. Delos et al. (1984) provide a procedure to estimate this rate. Where sedimentation is considered to be an important process, use a surface water fate model that has the capability of accounting for bed-water exchange and sediment load transport.

(3) Sorption
Substances dissolved in surface waters can sorb onto solids suspended in the water or onto bed sediments. This process, in effect, transfers the substances from the water to the sediment medium, and proceeds until an equilibrium point is reached. This equilibrium point (and the resulting water and sediment concentrations of the substance) is determined by the soil-water partition coefficient (a parameter that is a function of sediment type, water pH, cation exchange capacity, and organic content of sediment) and the physicochemical properties of the hazardous substance. In general, metals and hydrophobic, nonpolar organic compounds have a high tendency to sorb onto entrained or bottom sediment. See Lyman et al. (1982) for methods of estimating sediment adsorption of waterborne contaminants.

3.4.2.2 Intramedia Transformation Processes
The following is a brief description of the important intramedia transformation processes that may be significant for the surface water fate of hazardous substances. Rate-controlling factors are stated for each. Callahan et al. (1979), Mabey et al. (1982), Verschueren (1984), and Sax (1984) provide rate constants for these processes for numerous compounds.

(1) Photolysis
Chemical transformation due to photolysis utilizes energy from sunlight, and for some chemicals, can occur by several processes. Direct photolysis rates are a function of photon availability, light absorption coefficients for the chemical in question, and a reaction yield constant (i.e., the efficiency of substance transformation with the available solar energy). Indirect photolysis occurs through the action of intermediate substances naturally occurring in the medium. These intermediates absorb light energy by various processes and in this energized state, react with the hazardous substance. Indirect photolysis is a function of photon availability, concentration and light absorption coefficient of the intermediate, and a rate constant for the reaction between the energized intermediate and the hazardous material.

(2) Oxidation
Oxidation is the reaction of substances with oxidant species. Oxidation rates are a function of the concentrations of the substance in question, concentration of the oxidant, and a rate constant for reaction between them.

(3) Hydrolysis
Hydrolysis is the nucleophilic displacement of an electronegative substituent on a carbon atom by an hydroxyl group. The nucleophilic reactant can be either a water molecule or an hydroxyl ion. Hydrolysis of most compounds is highly dependent on the pH of the waterbody medium and can be promoted by both acid and base conditions. The rate of hydrolysis is a function of the concentration of the hazardous substance and the rate constants for the acid- and base-promoted processes at each pH value.

(4) Biodegradation
Biodegradation is the breakdown of substances through the enzymatic action of biota present in the water. Most biodegradation is carried out by microbial biota. It depends on the metabolic rates and characteristics and the population density of the biotic agents, which are in part functions of the availability of other nutrients, pH and temperature of the medium, and sunlight availability, among other factors.

3.4.2.3 Computer Models
Tables 3-5, 3-6, and 3-7 summarize the features, data requirements, resource requirements, and references or contacts for selected computer-based models appropriate to the in-depth analysis of the aquatic fate of hazardous releases from Superfund sites. Additional details for certain of the models addressed in the tables are provided below:

Exposure Analysis Modeling System (EXAMS-II) (Burns et al., 1982) is a steady-state and dynamic model designed for rapid evaluation of the behavior or synthetic organic chemicals in lakes, rivers, and estuaries. EXAMS-II is an interactive program that allows the user to specify and store the properties of chemicals and ecosystems, modify the characteristics of either via simple English-like commands, and conduct rapid, efficient evaluations of the probable fate of chemicals. EXAMS-II simulates a toxic chemical and its transformation products using second-order kinetics for all significant organic chemical reactions. EXAMS-II, however, does not simulate the solids with which the chemical interacts. The concentration of solids must be specified for each compartment; the model accounts for sorbed chemical transport based on solids concentrations and specified transport fields. Benthic exchange includes pore-water advection, pore-water diffusion, and solids mixing. The latter describes a net steady-state exchange associated with solids that is proportional to pore water diffusion.

A data set of average or typical values for waterbody-specific data is presently being developed by Battelle Northwest Laboratories, under contract to EPA. This data file will contain parameter values for a number of major U.S. river systems, lakes, and reservoirs, and will be integrated with the EXAMS program. These values will be accessible for fate modeling of the waterbodies included (GSC 1982).

MINTEQA1 (Felmy et al., 1984; Brown and Allison, 1987) is a geochemical model that is capable of

calculating equilibrium aqueous speciation, adsorption, gas phase partitioning, solid phase saturation states, and precipitation-dissolution of 11 metals (arsenic, cadmium, chromium, copper, lead, mercury, nickel, selenium, silver, thallium, and zinc). MINTEQA1 contains an extensive thermodynamic data base and contains six different algorithms for calculating adsorption. Proper application of MINTEQA1 requires applicable expertise, because kinetic limitations at particular sites may prevent certain reactions even though they might be thermodynamically possible.

Hydrological Simulation Program - FORTRAN (HSPF) (Johanson et al., 1984; Donigian et al., 1984) is a comprehensive package for simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants. HSPF incorporates the watershed-scale ARM (Agricultural Runoff Model) and NPS (Non-Point Source) models into a basin-scale analysis framework that includes pollutant transport and transformation in stream channels.

The model uses information such as the time history of rainfall, temperature, and solar radiation; land surface characteristics such as land use patterns and soil properties; and land management practices to simulate the processes that occur in a watershed. The result of this simulation is a time history of the quantity and quality of runoff from an urban or agricultural watershed. Flow rate, sediment load, and nutrient and pesticide concentrations are predicted. The program takes these results, along with information about the stream network and point source discharges, and simulates instream processes to produce a time history of water quantity and quality at any point in a watershed -- the inflow to a lake, for example. HSPF includes an internal data base management system to process the large amounts of simulation input and output.

Water Analysis Simulation Program (WASP4) (Ambrose et al., 1986, 1987) is a generalized modeling framework for contaminant fate and transport in surface water. Based on the flexible compartment modeling approach, WASP can be applied in one, two, or three dimensions. WASP is designed to permit easy substitution of user-written routines into the program structure. Problems that have been studied using WASP include biochemical oxygen demand, dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and toxic chemical movement.

A variety of water quality problems can be addressed with the selection of appropriate kinetic subroutines that may be either selected from a library or written by the user. Toxics WASP (TOX14; Ambrose et al., 1987) combines a kinetic structure adapted from EXAMS with the WASP transport structure and simple sediment balance algorithms to predict dissolved and sorbed chemical concentrations in the bed and overlying waters.

Eutrophication WASP (EUTRO4; Ambrose et al., 1987) combines a kinetic structure adapted from the Potomac Eutrophication Model with the WASP transport structure. EUTRO4 predicts dissolved oxygen, carbonaceous biochemical oxygen demand, phytoplankton, carbon, and chlorophyll a, ammonia, nitrate, organic nitrogen, and orthophosphate in the bed and overlying waters.

SARAH (Ambrose and Vandergrift, 1986) is a steady-state mixing zone model for back-calculating acceptable concentrations of hazardous wastes discharged to land disposal or waste water treatment facilities. For steady or batch waste streams, SARAH considers the following concentration reductions: dilution and loss during treatment, initial Gaussian mixing at the edge of a stream, lateral and longitudinal diffusion in the mixing zone, sorption, volatilization, hydrolysis, and bioaccumulation in fish. The user must specify, appropriate in-stream criteria for protection of the aquatic community, and humans through consumption of fish and water. The benthic community is not presently considered. Treatment loss is handled empirically. The human exposure pathways considered include ingestion of treated drinking water and consumption of contaminated fish.

3.4.2.4 Short- and Long-Term Concentration Calculations

Long-term average ambient water concentrations should be calculated using (1) the average release rate (from Chapter 3) projected for the time period of interest, and (2) the annual average stream flow rate as input to the above estimation procedures.

Short-term concentration levels are obtained through use of the short-term release rate developed during contaminant release analysis and the lowest reasonable 24-hour flow rate, or the 7-day, 10-year (7-Q-10) low flow rate for the period of record, as presented in the above estimation procedures.

Table 3-6 indicates several aquatic fate models capable of estimating both short- and long-term ambient water concentrations that are appropriate to in-depth analysis of the aquatic fate of contaminants released from Superfund sites.

3.5 Quantitative Analysis of Ground-Water Fate

To model the migration of contaminants in ground water the following factors should be estimated:

Table 3-5. Resource Requirements and Information Sources: Surface Water Fate Models

Model	Description	Resource Requirements, comments	References, sources of documentation, software
Water Quality Assessment Methodology (WQAM)	• Steady-state, 1-dimensional model • Requires only desk top calculations • Provides canonical information • Models lakes, rivers, and estuaries	• Easy to set up and use • No computer programming needed; requires only hand calculator • Recommended if time, costs, or information are restrictuve	*Reference*: Mills et al. 1982 *Documentation:* ORD Publications USEPA, Cincinnati, Ohio 45268 (513) 684-7562
Simplified Lake/Stream Analysis (SLSA)	• Steady-state, 1-dimensional model • Solution either by desk top calculations or simple FORTRAN program • Suitable for simplified lake and river systems	• Easy to set up and use • Computer programming not necessary; if used, only 280 bytes are required; suitable for microcomputers • Well documented and suggested for use before use of a more sophisticated model • May be used with hand calculator	*Reference*: HydroQual 1982 *Documentation:* William Gulledge 2581 M Street, N.W. Washington, D.C. 20037 (202) 887-1183
Michigan River Model (MICHRIV)	• Steady-state, 1-dimensional model • Computer program written in FORTRAN • Similar to SLSA, but can model more than one reach • Intended for metals • Models rivers and streams	• Easy to set up and use • Requires minimal computer programming	*Reference*: Delos et al. 1984 *Technical Assistance Available from*: Bill Richardson USEPA Environmental Research Laboratory - Duluth Large Lakes Research Station
Chemical Transport and Analysis Program (CTAP)	• Steady-state, 3-dimensional compartmental model • FORTRAN IV program suitable for numerous computers • Similar to SLSA except more sophisticated; each CTAP compartment is equivalent to one SLSA "lake" • Models streams, stratified rivers, lakes, estuaries, and coastal embayments	• Requires extensive data input • FORTRAN program - suitable for IBM 360/370, UNIVAC 108, CDC 6600 mainframe computers • Microcomputer version available requiring 32 K bytes storage • One of the better documented models, which may make it more desirable than other complex models	*Reference*: HydroQual 1982 *Documentation:* William Gulledge Chemical Manufacturers Association 2581 M Street, N.W. Washington, D.C. 20037 (202) 887-1183
Exposure Analysis Modeling System (EXAMS-II)	• Steady-state, 3-dimensional compartmental model • Complex computer program • Contains comprehensive second-order decay kinetics for organics; most models only have first-order kinetics • Models organic chemicals • Suitable for freshwater, non-tidal aquatic systems	• Requires extensive data input • Has been incorporated into EPA-OTS GEMS system (see Section 4.1) • Well documented and recommended for use over most other models • Available on magnetic tape for installation on mainframe or small computers (e.g., PDP-11 or HP 3000); batch version requires 64 K bytes memory at a minimum, more for complex modeling • Also available in interactive version, requiring 164 K bytes memory plus 2 K bytes for each chemical and 2.5 K bytes for each environment An estimated 350 hours required for installation and setup, assuming all data are readily available	*Reference*: Burns et al. 1982 *Documentation:* ORD Publications, Center for Environmental Research Information USEPA Cincinnati, Ohio 45268 (513) 684-7562 Center for Water Quality Modeling Environmental Research Laboratory USEPA Athens, Ga. 30613 (404) 546-3585

(Continued)

Table 3-5. (Continued)

Model	Description	Resource Requirements , comments	References, sources of documentation, software
Metals Exposure Analysis Modeling System (MINTEQAI)	• Steady-state, 3-dimensional compartmental model • Complex computer program • Designed for modeling of metal loadings • Suitable for freshwater, non-tidal aquatic systems	• Complex metal dynamics requiring extensive data input • Can be used with mainframe or small (e.g., PCP 11/70 or HP 3000) computers • Ineractive format • Contains data base with thermodynamic properties of 7 metals	*Further information*: Yasuo Onishi Battelle Pacific Northwest Laboratories Richland, WA 99352 (509) 376-8302
Hydrological Simulation Program - FORTRAN (HSPF)	• Time-varying, 1-dimensional model • Designed for year-round simulation • Models organic pollutants • Second-order decay mechanisms ○ Models non-tidal rivers, streams, and mixed lakes	• Requires extensive data input • Most suitable to minicomputers (e.g., HP 3000, PRIME, HARRIS) as model utilizes direct access input-output, which can be costly on mainframe computers ○ Requires 250 K bytes of overlay-type storage ○ Has been used on IBM 370 series computers	*Reference*: Johanson et al. 1984 *Software*: Center for Water Quality Modeling Environmental Research Laboratory USEPA Athens, GA 30613 (404) 546-3585
Transient One-Dimensional Degradation and Migration Model (TODAM)	• Time-varying, 1-dimensional model • Second-order decay mechanisms • Models river and estuarine systems ○ Requires exterior hydrodynamic model (e.g., EXPLORE) to provide channel and flow velocities to TODAM	○ Requires extensive data input • Complex FORTRAN program, written in the preprocessor language FLECS or in FORTRAN IV • Applicable to VAX or PDP 11/70 computers (batch mode) • TODAM has been applied; however, documentation is currently under review; release date unknown	*Reference*: Onishi et al. 1982 *Further information:* Yasuo Onishi Battelle Pacific Northwest Laboratories Richland, WA 99352 (509) 376-8302
Channel Transport Model (CHNTRN)	• Time-varying, 1-dimensional model • Models organic pollutants • Second-order decay mechanisms • Models rivers, lakes, estuaries, and coastal waters • Can be coupled with a hydrodynamic model, CHNHYD, to estimate flow dynamics where such data are not available	○ Requires extensive data input, and extensive setup time • Has not been field-tested, and documentation is currently under review • FORTRAN IV program language ○ Applicable to IBM 3933 computer, and others	*Reference*: Yeh 1982 *Documentation:* Dr.G. T. Yeh Environmental Sciences Division Oak Ridge National Laboratory P.O. Box X Oak Ridge, TN 37830 (615) 574-7285
Finite Element Transport Model (FETRA)	• Time-varying, 2-dimensional model (longitudinal and lateral) • Second-order decay mechanisms for organic pollutants • Models rivers, estuaries, coastal systems, and completely mixed lakes • Can be coupled with EXPLORE hydrodynamic model to generate flow velocities where these are unknown	• Input data requirements are extensive • Computer program written in FORTRAN IV • Can be used on IBM, VAX, or CDC-7600 computers • Has been field-validated • Setup and execution time requirements are extensive	*Reference*: Onishi 1981 *Further information:* Yasuo Onishi Battelle Pacific Northwest Laboratories Richland, WA 99352 (509) 376-8302

(Continued)

Table 3-5. (Continued)

Model	Description	Resource Requirements , comments	References, sources of documentation, software
Sediment-Contaminant Transport (SERATRA)	• Time-varying, 2-dimensional model (longitudinal and vertical) • Complex sediment transport mechanisms • Second-order decay mechanisms for organic pollutants • Models rivers and lakes	• Requires extensive data input • Computer program written in FORTRAN preprocessor language FLECS< in batch mode • Has been field-tested and is available for use • Requires an estimated 750 man-hours for setup, assuming all required data are readily available	Reference: Onishi and Wise 1982a, Onishi and Wise 1982b *Documentation:* ORD Publications Center for Environmental Research Information USEPA Cincinnati, OH 45268 (513) 684-7562 *Technical Assistance:* Robert Ambrose EPA Athens Environmental Research Lab Center for Water Quality Modeling Athens, GA 30613 (404) 546-3546
Estuary and Stream Quality Model (WASP4)	• Time-varying, 3-dimensional model • Sophisticated second-order organic decay kinetics • Models rivers, lakes, and estuaries	• Very data-intensive model • User must provide hydrodynamic flows between model compartments • Applicable to IBM 370 or PDP 11/70 systems • FORTRAN IV program requires 64 K bytes memory • Requires 150-300 man-hours for setup	*Documentation and Software:* Dr. John Connolly Environmental Engineering and Science Manhattan College Bronx, N.Y. 10471 (212) 920-0276 *or:* Dr. Parmely H. Prichard Environmental Research Laboratory Gulf Breeze, FL 32561 (904) 932-5311 Robert Ambrose Center for Water Quality Modeling USEPA Athens, GA 30613 (404) 546-3546
Surface Water Back Calculation Procedure (SARAH)	• Steady-state, 1-dimensional analytical solution • FORTRAN Code • Models contaminated leachate plume feeding the downgradient surface waterbody (stream or river) • Monte Carlo simulated generic environment • Degradation, dilution, sorption, and volatilization • Bioaccumulation in fish	• Generic environment, minimal data input • FORTRAN model	*Documentation:* Jan. 14, 1986 *Federal Register,* Hazardous Waste Management System, Land Disposal Restrictions, Proposed Rule *Software:* , David Disney, Environmental Research Laboratory, Environmental Protection Agency, College Station Road, Athens, GA 30613, (404) 546-5432, or (404) 546-3123

Source: Versar 1983a.

Table 3-6. **Features of Surface Water Fate Models**

	STREAMS/RIVERS	IMPOUNDMENTS	ESTUARIES/TIDAL	1-DIMENSIONAL	MULTIDIMENSIONAL	ACCOUNTS FOR DISPERSION	ACCOUNTS FOR BIODEGRADATION	ACCOUNTS FOR PHYSICAL REMOVAL	HANDLES VARYING STRATIFICATION	HANDLES VARYING RELEASE RATES	HANDLES DYNAMIC WATER FLOW	STEADY STATE	POINT SOURCE	NONPOINT SOURCE	ORGANIC POLLUTANTS	METALS/INORGANICS	PARTICULATE POLLUTANTS	PREDICTS CONTAMINANT CONCENTRATION AS A FUNCTION OF DISTANCE FROM SOURCE	PREDICTS METAL SPECIATION	PREDICTS BIOCONCENTRATION OF CONTAMINANTS	PREDICTS LONG-TERM AVERAGE LEVELS OF CONCENTRATIONS AT RECEPTORS	PREDICTS SHORT-TERM MAXIMUM CONCENTRATIONS FOLLOWING TERMINATION OF RELEASE	PREDICTS PERSISTENCE OF CONTAMINANT AT RECEPTORS	
QUAL2	◐	◐	◐	◐			◐	◐	◐			◐	◐	◐	◐	◐	◐	◐	◐			◐		
SLSA	◐	◐		◐			◐	◐		◐		◐	◐		◐	◐	◐	◐	◐			◐	◐	◐
MICHRIV	●			●			◐	●				●	●		●	●	●	●				◐		
CTAP	◐	◐	◐		◐	◐	◐	◐	◐			◐	◐		◐	◐	◐	◐				◐		
EXAMS II	◐	◐		◐	◐	◐	◐	◐	◐	◐		◐	◐	◐	◐		◐	◐		◐	◐	◐	◐	◐
MINTEQA 1	◐	◐										◐				◐	◐		◐					
HSPF	◐	◐		◐			◐	◐		◐	◐		◐	◐	◐	◐	◐	●				◐	◐	◐
TODAM	●		●	●		●	◐	◐		●	●		●	●	●	●	●	◐				◐	●	●
CHNTRN	●	●	●	●		●	●	●	●	●	●		●	●	●		●	●	●			●	●	●
FETRA	●	●	●	●	●	●	●	●		●	●		●	●	●	●	●	●				●	●	●
SERATRA	●	●			●	●	●	●	●	●	●		●	●	●	●	●	●				●	●	●
WASP 4	●	●	●	●	●	●	●	●	●	●	●		●	●	●			●				●	●	●
SARAH	●			●		●	●	●				●	●	●	●	●	●	●		●	●	●		

Sources: USEPA 1985h; Delos et al. 1984

Table 3-7. Data Requirements for Surface Water Models

	WATER BODY PHYSIOGRAPHY	FLOW RATES	WATERSHED LAND USE/CHARACTERISTICS	CLIMATIC DATA	WATER BODY BIOLOGICAL PARAMETERS	WATER PHYSICAL PROPERTIES (e.g. TEMPERATURE, ETC.)	WATER CHEMICAL PROPERTIES	ESTUARY SALINITY PROFILES	SEDIMENTATION/RESUSPENSION VELOCITIES	SEDIMENT BED DEPTHS	SEDIMENT BED OM CONTENT PARAMETERS	OVERALL AQUATIC HALF-LIFE VALUES	SUBSTANCE PHYSICAL/CHEMICAL PROPERTIES	DISPERSION COEFFICIENTS	CHEMICAL PARTITION COEFFICIENTS	WATER COLUMN DEGRADATION COEFFICIENTS	BED SEDIMENT DEGRADATION COEFFICIENTS	AVERAGE RELEASE RATES	DYNAMIC RELEASE PATTERNS
WQAM	●	●	●					●				●		●	●	●		●	
SLSA	●	●							●	●					●	●	●	●	
MICHRIV	●	●													●	●	●	●	
CTAP	●	●							●	●	●		●		●	●	●	●	
EXAMS II	●	●		●	●	●	●			●	●	●	●	●	●	●	●	●	●
MINTEQA 1						●	●							●	●			●	
HSPF	●	●	●	●	●	●	●		●	●	●	●		●	●	●	●	●	●
TODAM	●	●							●		●		●	●	●	●	●	●	●
CHNTRN	●	●		●	●	●	●		●		●	●	●	●	●	●	●	●	●
FETRA	●	●							●		●		●		●	●	●	●	●
SERATRA	●	●							●		●		●		●	●	●	●	●
WASP 4	●	●		●	●	●	●		●	●	●	●	●	●	●	●	●	●	●
SARAH		●		●	●	●	●					●	●	●	●	●		●	

Sources: USEPA 1985h; Delos et al. 1984

Direction - The direction of contaminant migration is important in predicting the potentially exposed population.

Velocity - The migrating contaminant's velocity is important in assessing when contamination will reach the exposed population and how long the contamination will be affecting that population.

Concentration - Concentration of the contaminant in ground water at the exposure locations is used to calculate dose to the population. This factor is used to convert the amount of water consumed each day to the mass of contaminant received each day. The mass information is then used to predict health effects associated with exposure to the contaminant (USEPA 1985d).

Volume - The contaminated region's volume is important in evaluating the extent of the contamination, which is essential to estimating costs of remedial measures and viability of specific alternative remedial measures for the particular site. It is also useful for determining how long a remedial measure will have to be taken.

The following ground-water discussions are divided into three sections:

1. The minimum technical foundation that is needed in order for the analyst to apply and interpret the equations and models for ground water. This discussion is meant to support the hydrologist familiar with water supply calculations, providing an introduction to contaminant hydrology. Readers needing a more complete introduction to hydrology may wish to read EPA's Handbook titled "Groundwater" (EPA/625/6-87/016).

2. Equations that can predict average contaminant velocity and mass flux for dilute solute and concentrated contaminant plumes. Knowing the travel time and the degradation half-life, one can predict contaminant attenuation. A nomograph is provided for predicting dilution and contaminated front velocity of dilute solute plumes, as are equations that are useful in assessing the extent of contamination. The narrative contains guidance for interpreting available monitoring data from existing wells and from monitoring wells. All of the equations apply to homogeneous and isotropic media; fractured rock flow and karstic terrain flow are not addressed.

3. Computer models that predict dilution, attenuation, and contaminated front velocity of dilute solute plumes only. All of the computer models assume homogeneous and isotropic media. Computer models that predict organic fluid migration are not discussed, nor are models that describe karstic terrain flow. The state of the art for these models is not well-developed, and thus they are considered beyond the scope of this report. The analyst wishing to model organic fluid migration in porous media should use the equations in Section 3.5.2.

3.5.1 Discussion of Ground-Water Modeling

3.5.1.1 The Contamination Cycle

The two primary types of ground-water contamination at uncontrolled hazardous waste sites involve leaching of solid contaminants and percolation of liquid contaminations to the underlying aquifer. Solid material itself does not generally contaminate ground water directly, because it does not move through the porous soil. Thus, it will not migrate until precipitation (or ground water) leaches (dissolves) some of it and carries it down to the water table. Ground-water contamination by this route depends on the precipitation rate and the solubility of the solid contaminant. A variation of this route involves dissolution of the solid contaminant by a complex leachate that contains organic constituents as well as water. The existence of dissolved organic constituents in the leaching fluid causes organic contaminants to have a higher solubility. The importance of this phenomenon is greatest for contaminants with a high octanol/water partition coefficient (Enfield 1984, Jaw-Kwei n.d.).

Liquids do not need infiltrating precipitation to carry them down to the water table; they move on their own with help from gravity. Thus, ground-water contamination by liquids is not dependent on the precipitation rate or the solubility of the contaminant. The viscosity and density of a liquid affect its rate of migration. After the liquid has percolated through the soil, some will remain in the interstitial pore spaces; this material will dissolve into the percolating precipitation and migrate downward as a function of its water solubility and the rainfall rate. Another source of contamination by liquid material arises from intentional injection into the aquifer itself (deep-well injection) or "injection" into the vadose (unsaturated) zone (unlined lagoons).

Hazardous waste is often assumed to be primarily solid waste; however, studies showing the relative proportion of solid to pourable hazardous RCRA wastes indicate that pourable hazardous waste constitutes 60 to 95 percent of the total (Skinner 1984). The equations for modeling liquid waste migration pertain to a larger percentage of the waste migration situations than the dilute solute transport models (computer models/nomograph).

Two other types of ground-water contamination may also occur. These are contamination by gaseous contaminants and contamination by intermedia transfers. Gases constitute a relatively small source of ground-water contamination, since they are more

likely to contaminate air than ground water. The main mechanism for gases contaminating ground water is equilibration of gases leaking from buried containers or injected into the ground, with percolating rainwater causing subsequent downward migration and mixing of this contaminated water with ground water. Intermedia contamination of ground water can come from either air or surface water. Contamination from air can result from two mechanisms: rain-out and wash-out. Rain-out occurs when airborne contaminated particulates form condensation nuclei for the formation of rain drops. Wash-out occurs when falling rain captures gaseous or particulate contaminants as it falls to earth. The concentrations of contaminants entering ground water as a result of gaseous contamination or intermedia transfers are generally very small, and these are not considered to be significiant sources of ground-water contamination in most cases.

A third source of contamination that may be significant at some sites is through ground-water/surface-water system interconnections. That is, contaminated surface water may recharge a ground-water system. This occurs only in reaches where the surface-waterbody is a "losing stream" (i.e., one that supplies water to the ground-water system). Frequently, ground water feeds surface water (gaining reaches). For gaining reaches, the ground water, if contaminated, contaminates the surface-waterbody into which it discharges.

One aspect of the contamination cycle that should be considered is the ratio of contaminant to contaminated ground water. A very small quantity of concentrated contaminant can contaminate a large volume of ground water to the ppm or ppb level.

3.5.1.2 Ground-Water Flow Conditions

After precipitation infiltrates the surface of the ground, it travels vertically down through the vadose zone (unsaturated zone) where it meets the water table, and it then flows approximately horizontally. The horizontal flow within the aquifer is saturated.

(1) Saturated Zone

A simplified flow equation is used to describe the volumetric flow of water through a porous medium under saturated conditions. The volumetric flow (or discharge) is proportional to the product of the driving force, the soil's ability to transmit water, and the cross-sectional area perpendicular to the flow direction. The driving force is the difference in the energy (hydraulic head) between two points in the aquifer divided by the distance between the two points. This driving force is called the hydraulic gradient. A soil's ability to transmit water is represented by an empirically determined coefficient of hydraulic conductivity. This equation is called Darcy's law. The properties of the liquid (water or contaminant) and the permeability of the porous medium determine the hydraulic conductivity. The soil has an intrinsic property of permeability, which is determined by the size, orientation, and connectedness of the pore spaces.

Soil permeability is a function of soil pore space, which is determined by soil particle size. Small diameter clay soil particles cause clay soil to have low permeability, while larger diameter sandy soil particles result in the high permeability of sandy soils. The permeability, and therefore the hydraulic conductivity, of a homogeneous soil is constant under conditions of saturated flow.

In cases where the vadose zone is saturated and the flow direction is vertical, the change in height of the water per unit of vertical travel distance is always one. Thus, the hydraulic gradient for vertical saturated flow is unity, and the volumetric flows are proportional to the permeability alone.

(2) Unsaturated Zone

Darcy's law governs flow anywhere in the porous medium, including the vadose, or unsaturated, zone. In the vadose zone, however, the pore spaces are not saturated with water or any other liquid. The hydraulic conductivity of any liquid through a porous medium is partly dependent on the amount of liquid in the pore spaces, and hydraulic conductivity for unsaturated soil can be expressed as a fraction of the hydraulic conductivity at saturation.

When the pore spaces are entirely filled with liquid (i.e., saturated), the hydraulic conductivity for that medium is at its maximum value. This is called the saturated hydraulic conductivity (or simply hydraulic conductivity), and it is essentially constant for a specific liquid saturating a specific soil medium.

The unsaturated hydraulic conductivity at residual moisture content is very small. When the soil is very dry, most of the moisture is tightly bound by capillary forces in the void spaces, and the water will not flow easily. Unsaturated hydraulic conductivity increases, gradually at first and then more rapidly, as the degree of saturation increases from the residual moisture content to the saturated moisture content. Since the hydraulic conductivity is dependent upon the moisture content, the specific discharge through the vadose zone varies with the degree of saturation at any depth.

The rate of infiltration at the ground surface may be limited by the capacity of the soil to accept water or by the delivery rate of water at the ground surface (e.g., the precipitation rate). The infiltration rate into soil cannot exceed the value for that soil's saturated hydraulic conductivity. When the hydraulic loading to the surface of the ground is low, such as light rainfall alone, the flow of water through the vadose zone is

unsaturated; however, when the hydraulic loading is large, such as beneath a lagoon, the flow of water through the vadose zone can be saturated. When the hydraulic loading is small, it is limiting and the vertical flow through the vadose zone is unsaturated. When the hydraulic loading is larger than the flow that can move through the soil with saturated flow, the permeability of the soil is limiting the flow, and the vertical flow through the vadose zone is saturated.

3.5.1.3 Multiphase Flow

The water solubility of any particular chemical will determine whether it will be transported as a solute, as a colloid, or as a separate, concentrated phase. Many chemicals that have been identified as contaminants in ground water are sparingly soluble in water. When introduced to the ground-water system as liquids, such chemicals can flow as an independent species through the porous medium. When the immiscible contaminant comes into contact with the water in the pore spaces of the vadose zone or at the water table (phreatic surface), the liquids do not mix but essentially remain as two separate phases. Some of the chemical will go into solution with the water, but since the solubility of the chemical is very low, the bulk of the contaminant will remain as a separate layer that could saturate the pore spaces it is flowing through. Thus, the migration of two immiscible liquids in porous media is called two-phase flow.

Complete descriptions of two-phase flow require an additional equation for each separate phase present in the flow system. Several general rules that can be applied in analyzing ground-water contamination problems involving immiscible chemicals, are as follows:

(1) Floaters

The specific gravity of an immiscible liquid contaminant will determine whether water will displace it or it will be displaced by water. In downward flow, water can displace the lighter, immiscible liquid so the water is found below the immiscible liquid. In horizontal flow, the less dense, immiscible liquid will tend to float upward until the separate immiscible phase floats on top of the water table. Thus, the immiscible liquids that have a specific gravity of less than one are sometimes referred to as "floaters." As a general rule, immiscible hydrocarbons that are nonchlorinated are floaters (less dense than water).

(2) Sinkers

Immiscible contaminants more dense than water, whose specific gravity values are greater than one, can displace water when flowing through the porous medium. Gravity will cause dense immiscible liquids to sink as they flow horizontally through the porous medium. Thus, the immiscible liquids more dense than water are often referred to as "sinkers." Generally, chlorinated hydrocarbons that contaminate water are more dense than water.

Density and specific gravity are intrinsic properties of a chemical, and values for natural or manufactured chemicals are usually published (Verschueren 1984; Callahan et al. 1979).

(3) Hydraulic Gradient for Immiscible Fluids

The hydraulic gradient, the difference in the hydraulic heads at two points divided by the distance (along the flow path) between the points, is the driving force for ground-water movement in a porous medium. With regard to an immiscible separate phase, however, the gradient that causes the immiscible liquid to flow is not necessarily the same as that which influences the ground water. If contaminants in an immiscible phase that is more dense than water reach the bottom of the aquifer, that separate phase may alter its flow direction to conform to the shape and slope of the aquitard surface. In some cases, the base of the aquifer may be sloped in a different direction from the direction of flow determined by the hydraulic gradient. This possibility should be considered when the analyst tries to identify the direction of the contaminant plume's migration.

The assumption that the hydraulic gradient of the separate, immiscible phase approximates that of ground water is quite reasonable for the less dense immiscible liquids. Since these contaminants float on the water table, the hydraulic gradient of the phreatic surface is probably also the gradient of the immiscible phase.

(4) Hydraulic Conductivity of Immiscible Fluids

If the saturated hydraulic conductivity of water through a porous medium is known, it is very easy to modify that value to calculate the hydraulic conductivity of that same porous medium saturated with a different liquid, such as a separate layer of an immiscible phase.

3.5.1.4 Contaminant Flow and Hydrodynamic Dispersion

In contaminant transport, contaminants can be thought of as a mass flowing through a cross-sectional area of the porous medium that is perpendicular to the flow direction. The discussion presented here is for solute transport (mass that is transferred with the flowing ground water), but basic concepts also apply to the flow of immiscible, separate phases.

The movement of contaminants in ground water can be described by two principal mechanisms: gross fluid movement (advective flow) and dispersion. Gross fluid movement can be either ground-water movement or organic fluid movement (the waste itself moving as a concentrated liquid). Dispersion also can be described by two principal mechanisms: fluid

mixing (mechanical dispersion) and diffusion. The next section addresses the underlying mechanisms for fluid mixing.

Fluid mixing is important for two reasons: (1) precise modeling of contaminant movement and (2) modeling of dilution of the contaminant concentration between source and exposed population.

Dilution (mixing) in ground water is different from dilution in air and in surface water. In both air and surface water, dilution is a major phenomenon. In ground water, the magnitude of dilution is much smaller. Flow in both air and surface water can be turbulent. Turbulent flow means that all the flow paths are not essentially parallel to the gross direction of motion; some flow paths are at right angles to the bulk fluid motion. The flow components that are perpendicular to the bulk fluid motion cause the plume to spread laterally. This reduces the concentration in the plume, while making the plume contaminate a larger volume of air or surface water.

In ground water, turbulent flow rarely exists. The slow speed of ground water coupled with the straightening effect of many soil particles keeps the flow smooth and laminar. In an idealized conceptual model, the interconnecting pore spaces can be thought of as forming flow channels or tubes; any tendency for the flow to eddy is resisted by the sides of the flow channel. Since the interconnecting pore spaces do not make a continuous flow channel, some lateral mixing will occur in real soil.

Dispersion in air and surface water is caused by the eddy currents (and diffusion). If the flow is broken up into two components, longitudinal flow and eddy flow, the gross motion is due to the longitudinal flow, and the eddy flow is responsible for mixing. The magnitude of the eddy currents is the same in all directions (longitudinal, transverse, and vertical). Since the concentration gradients are weaker in the longitudinal direction than they are in the transverse and vertical directions (for continuous steady state sources), the net effect of mixing in the longitudinal direction is small compared to the effect of mixing in the directions perpendicular to the flow direction. When air and surface water are modeled, the longitudinal mixing is often neglected; lateral mixing is modeled as the principal mixing phenomenon.

Dispersion in ground water is not caused by eddy currents. Dispersion (neglecting diffusion for the moment) is caused by four principal phenomena: varying pore sizes, varying path length, variation in velocity gradient across pore space, and flow splitting around soil particles with mixing within the pore space. The first three phenomena contribute to longitudinal dispersion; the last phenomenon causes lateral dispersion. In ground water, the magnitude of the mixing is much greater for longitudinal mixing than for lateral mixing. Researchers have reported longitudinal dispersivity values ranging from 2 to 25 times higher than transverse dispersivity values (Gelhar et al. 1985).

In ground water, dilution occurs at a much slower rate than it does in air or surface water. The overall magnitude of mixing is smaller, and the component of mixing that is most important to dilution (lateral) is the smaller component of ground-water mixing. For short-term releases (spills), longitudinal mixing is useful in diluting plume concentrations. This is because the plume can effectively mix with the uncontaminated water in front of and behind the slug of contamination, whereas continuous sources make the length of the plume so long that its middle section cannot effectively mix with clean water in front or behind it.

3.5.1.5 Transformation and Retardation

Movement of contaminants can be modeled by fluid movement, fluid mixing, and diffusion; however, for more accurate modeling, chemical transformation and retardation should also be considered. Some contaminants are subject to transformation and retardation while others are not; the relative significance of transformation and retardation for specific contaminants determines the need to model these mechanisms. Transformation is the term used to describe loss of the contaminant from the plume. The mass of the contaminant is not lost; rather, the molecular structure is changed so that the toxicity associated with the initial molecular structure is no longer present. When the molecular structure of degradation products is more toxic than the original contaminant, degradation is not considered attenuation. Attenuation is used to describe chemical structure changes that reduce or eliminate the toxicity of the contaminant, and to describe phenomena that function as sinks for toxic contaminants. Phenomena that are reversible are not sinks for toxic contaminants.

Chemical interactions between contaminants and the soil matrix that are reversible delay the migration of contaminants but do not act as a sink. The effect of these chemical interactions is modeled as retardation. Retardation is modeled using a coefficient to scale down the velocity of ground water to the slower effective velocity of the contaminant mass. Attenuation reduces population risk; retardation delays population risk.

Many reversible interactions can cause retardation phenomena; however, only two retardation mechanisms apply to wide classes of contaminants and are well enough understood to be modeled on a regular basis. Organic retardation and cationic retardation are the most frequently modeled phenomena. Organic retardation refers to hydrophobic contaminants sorbing onto organic material in the soil

matrix. Cationic retardation refers to positive charged ions associating with the soil matrix. This association can be due to polar species in the ground water being attracted to the ionic double layer surrounding clay particles in the soil, or it can be due to ionic bonding with the soil matrix.

(1) Retardation of Organics
Organic retardation, which refers to hydrophobic contaminants sorbing onto organic material in the soil matrix, is estimated in ground water by the use of a retardation coefficient. The velocity of each compound in ground water is a function of the characteristics of the soil media and the compound's octanol-water partition coefficient. The octanol-water partition coefficient measures the compound's degree of hydrophobicity. The parameter of the soil media that determines the presence of sorption sites is the percent of organic carbon in the soil.

When the contaminant concentration in the water is high and the quantity of contaminant on the surface of the soil organic carbon is low, the net transfer is from the water to the soil. Since the transfer is an equilibrium process, it reverses when the concentration in the water is low and the quantity of contaminant on the surface of the soil organic carbon is high.

If the leachate contains sufficient quantities of organic material to affect the solubility of the contaminant, the modeling of retardation is more difficult. The toxic constituent flow will still be retarded, but not as much. Instead of partitioning between the water and soil organic carbon, the contaminant will partition between the polar-organic fluid and the soil organic carbon. The toxic contaminant will spend a smaller fraction of time on the solid soil particles and a larger fraction of time in the fluid; this will increase its migration velocity. Modeling this phenomenon, however, is complex and has already been well documented elsewhere. The analyst interested in modeling retardation in complex leachates is referred to Nkedi-Kizza et al. (1985), Rao et al. (1985), and Woodburn et al. (1986).

Once a contamination source stops contaminating the ground water (either a one-time slug or the end of a long-term loading), the saturated sorption sites start to lose contaminants to the clean ground water that flows after it. This phenomenon causes the development of a plume shape that has a long tail of decreasing contamination. Since the rate of desorption is high when the degree of saturation is high, and is lower as the quantity of contaminant on the sorption sites diminishes, the desorption phenomenon can provide a degrading influence on the ground water for a long time.

(2) Retardation of Cations
In cationic retardation, positively charged ions associate with the soil matrix (clay particles). There is a smaller effect for anion exchange. Anion exchange is due to positive charges associated with hydrous oxides. Since soils typically have more negatively charged clay particles than positively charged hydrous oxides, cations flow with a more retarded velocity than do anions. Contaminants that are not charged are not subject to ionic retardation. Contaminants that are compounds or complexed ions also are not retarded by ionic retardation.

Cationic retardation is reversible, as is organic retardation, and it forms a trail of low-level contamination after the source of contamination stops. Once a source stops contaminating the ground water, the saturated ion exchange sites start to lose contaminants to the clean ground water. This phenomenon causes the development of a plume shape that has a long tail of decreasing contamination. Since the rate of release is high when the degree of saturation is high, and lower as the quantity of contaminant on the ion exchange sites diminishes, the reversible ion exchange phenomenon can provide a degrading influence on the ground water for a long time.

(3) Transformation/Attenuation
Transformation/attenuation is the term used to model sinks for contaminants. The particular type of chemical fate modeled depends on the contaminant and the soil characteristics. The following is a list of different fate mechanisms:

- Hydrolysis
- Complexation-chelation
- Acid/base reactions
- Oxidation/reduction reactions
- Biodegradation
- Radioactive decay
- Chemical precipitation
- Coagulation
- Peptization reactions.

Attenuation is modeled with the use of a "half-life" parameter. Whether the degradation is due to hydrolysis or biodegradation, the time necessary for the concentration to drop by half is the measure of degradability.

Appropriate individual decay rates or overall decay coefficients have been developed for some substances and are available in the technical literature. Sources for such data include: Callahan et al. (1979); Dawson et al. (1980); Mabey et al. (1982); Sax (1984); USCG (1974); and Verschueren (1984). Methods of estimating decay coefficients are presented by Lyman et al. (1982).

3.5.1.6 Higher Velocity Transport

Some situations can cause the migration velocity of contaminants to be faster than the ground-water velocity. Macromolecules can themselves move faster than the ground water, and any hydrophobic contaminants that are sorbed onto them will also move faster. Until recently, hydrophobic contaminants were thought to flow with a retarded velocity only because of preferential sorption onto stationary organic soil particles. In such cases, the time the contaminant spends on the stationary soil particles lowers its average velocity. Conversely, the time a contaminant spends on a "high speed" macromolecule raises the average velocity of the contaminant. Since hydrophobic contaminants sorb onto both stationary and higher velocity macromolecules, both must be considered in order for the modeling of transport for hydrophobic contaminants to be complete.

Macromolecules may be found in ground water in concentrations ranging from 1 mg/l to 10 mg/l and are large enough that only the large pore spaces are available for migration. This means that their average velocity is the average velocity of the large pore spaces, and not the average velocity of all the pore spaces. The velocity of flow through each pore space is a function of the size of the pore space, and the larger pore spaces allow faster flow than do the small spaces. The velocity difference between the average large pore space and the average pore space is approximately one order of magnitude.

Macromolecules with large hydrophobic surface area and small polar surface area will flow with a retarded velocity because of reversible sorbtion onto soil carbon. These macromolecules will not cause higher speed transport. Macromolecules with large polar surface areas and small hydrophobic surface areas will travel faster than the ground water. These molecules can speed up the migration velocity of hydrophobic contaminants.

Macromolecular transport is not frequently modeled; however, when such modeling is necessary, the analyst can refer to Enfield and Bengtsson (n.d.) for detailed guidance.

3.5.2 Ground-Water Modeling Equations and Nomograph

This section provides a number of hydrologic modeling equations and a nomograph. In no cases will all equations be necessary; depending on the observed chemical contaminant, a discrete subset of the equations will be useful in assessing the ground-water contamination problem at a specific uncontrolled hazardous waste site.

Five discrete classes of contaminant are discussed. Each class is based on a different technique for calculating contaminant migration. The five classes of contaminant can have dramatically different calculated velocities and concentrations; use of the appropriate analytical techniques for each class is thus necessary for accuracy.

Estimating contaminant velocity is based on estimating water velocity. For those contaminants that flow as water flows, contaminant velocity equals water velocity (vertical or horizontal). For those that flow at rates different from water, the estimated water velocity must be adjusted to approximate that of the contaminant.

3.5.2.1 Calculating Ground-Water Velocity

Ground-water velocity can be determined for both the saturated zone and the vadose (unsaturated) zone. Vadose zone velocity is discussed in the next section; saturated zone velocity is discussed in this section.

Ground-water velocity in the saturated zone is calculated using Darcy's Law (Bouwer 1978):

$$v = K_s i \qquad (3\text{-}9)$$

where

- v = Darcy velocity of water, also termed superficial velocity, or specific discharge, (length/time).
- K_s = hydraulic conductivity of soil or aquifer material, (length/time).
- i = hydraulic gradient, (length/length).

However, v, the Darcy velocity, is not the real macroscopic velocity of the water, but the velocity as if the water were moving through the entire cross-sectional area normal to the flow, solids as well as pores (Bouwer 1978). The ground-water velocity is calculated from the Darcy velocity by dividing it by soil porosity, or, for more precise modeling, by effective porosity (thus taking into account the fact that the entire cross-section of the pore is not flowing (i.e., due to boundary layer effects). For clay soils, the effective porosity also corrects for the effect of electro-osmotic counterflow and the development of electrokinetic streaming potentials (Bouwer 1978). The equation for calculating ground-water velocity from Darcy velocity using effective porosity is as follows (Bouwer 1978):

$$v_{pw} = v/P_e \qquad (3\text{-}10)$$

where

- v_{pw} = ground water (pore water) velocity, (length/time).
- v = Darcy velocity (superficial velocity, specific discharge), (length/time).

P_e = effective porosity, (dimensionless fraction).

The above terms should be determined for the site being studied. If this is not possible for all parameters, then literature values can be used for the few parameters that are not available. Literature values for saturated hydraulic conductivity are presented in Table 3-8 (Rawls et al. 1982) and Table 3-9 (Freeze and Cherry 1979).

The hydraulic gradient (the change in the elevation of the water table over distance from the site) should also be taken from field data developed during site investigation. Water levels in existing nearby wells can also provide an indication of hydraulic gradient. Table 3-10 provides values for saturated moisture content, which is roughly equal to the effective porosity, or P_e, for several soil types.

It must be emphasized that site-specific data are highly preferable to regional data, or data obtained from any of the above-referenced tables. If site-specific information on effective porosity is available, it should be used; however, literature values for soils with the same hydraulic conductivity provide sufficient accuracy. Effective porosity (P_e) can be approximated by the difference between the moisture content at saturation and at the wilting point (-15 bar)*. The equation is as follows (Rawls 1986):

$$P_e = \theta_s - \theta(-15) \qquad (3\text{-}11)$$

where

P_e = effective porosity, (fraction, dimensionless).
θ_s = water content when the pores are fully saturated, (fraction, dimensionless).
$\theta(-15)$ = wilting point moisture content, (fraction, dimensionless).

This estimation procedure addresses the fraction of the pore spaces that is contributing to flow, but does not address the effect of electro-osmotic counterflow and the development of electrokinetic streaming potentials. For clays, this can be a significant difference. Literature values listed in Table 3-10 should be used for clay solids (these values incorporate the effects of the clays ionic double layer) (Rawls et al. 1982); either technique can be used for sand or loam soil.

The above method for predicting the average velocity of ground water is the most widely accepted approximation; however, it is only an approximation and further refinement of this approach would improve accuracy. Corrections for the path length difference between the straight line distance versus the tortuous path through which ground water flows can improve the precision (Freeze and Cherry 1979), although the literature does not provide a consistent correction factor to apply. To provide a feel for the magnitude of this correction, the analyst can review Das (1983) which suggests a correction of 1.41. This value can be used to correct the velocity or the distance (not both) by dividing the number by 1.4. However, the analyst must interpret the results obtained through such correction with care, as the degree to which the factor cited in Das applies to any given site is uncertain.

*Wilting point is determined by drawing a suction of -15 bar to draw water out of the soil in a manner similar to the suction of a plant root. Bar is a measure of pressure (dynes/cm^2).

3.5.2.2 Calculating the Velocity of Infiltrating Rainwater

This section discusses the calculation of the velocity of percolating rainwater flowing through the vadose zone. Darcy's law can be used to calculate the unsaturated flow velocity; however, the hydraulic conductivity must be corrected to reflect the effect of partially-filled pore spaces when the hydraulic loading is below that necessary to support saturated flow.

Interstitial pore water velocity for unsaturated transport through the vadose zone can be calculated as follows (Enfield et al. 1982):

$$v_{pw} = q/\Theta \qquad (3\text{-}12)$$

where

v_{pw} = interstitial ground water (pore water) velocity, (length per unit time).
q = average percolation or recharge rate, (depth per unit time).
Θ = volumetric moisture content of the unsaturated zone, (decimal fraction, representing volume of water per volume of soil).

This equation applies to steady-state conditions, or those that can be assumed to be steady. For unsteady hydraulic loading, the "q" and "Θ" will vary with time and depth. Additionally, the distribution of "q" and "Θ" will vary as the moisture migrates down. This makes determination of the average transport velocity burdensome. For situations where steady-state conditions cannot be assumed, the analyst should use a computer model; for example, SESOIL (one of EPA's GEMS computer system) calculates the time of travel for seasonally varying rainfall rates.

The volumetric water content (Θ) in the unsaturated zone can be estimated using the following equation (Clapp and Hornberger 1978):

Table 3-8. Representative Values of Saturated Hydraulic Conductivity

Soil texture	Number of soils[a]	Hydraulic conductivity (K_s; cm/sec)[b]
Sand	762	5.8×10^{-3}
Loamy sand	338	1.7×10^{-3}
Sandy loam	666	7.2×10^{-4}
Loam	383	3.7×10^{-4}
Silt loam	1,206	1.9×10^{-4}
Sandy clay loam	498	1.2×10^{-4}
Silt clay loam	366	4.2×10^{-5}
Clay loam	689	6.4×10^{-5}
Sandy clay	45	3.3×10^{-5}
Silt clay	127	2.5×10^{-5}
Clay	291	1.7×10^{-5}

[a]Number of individual soil samples included in data compiled by Rawls et al. 1982.
[b]Predicted values based on compiled soil properties.
Source: Adapted from Rawls et al. 1982.

Table 3-9. Saturated Hydraulic Conductivity Ranges for Selected Rock and Soil Types

Saturated Hydraulic Conductivity (cm/sec)

Soils			
Unweathered marine clay	5×10^{-11}	--	10^{-7}
Glacial till	10^{-10}	--	10^{-4}
Silt, loess	10^{-7}	--	10^{-3}
Silty sand	10^{-5}	--	10^{-1}
Clean sand	10^{-4}	--	1
Gravel	10^{-1}	--	10^{2}
Rocks			
Unfractured metamorphic and igneous rock	10^{-2}	--	10^{-8}
Shale	5×10^{-12}	--	10^{-7}
Sandstone	10^{-8}	--	5×10^{-4}
Limestone and dolomite	5×10^{-8}	--	5×10^{-4}
Fractured igneous and metamorphic rock	10^{-6}	--	10^{-2}
Permeable basalt	10^{-5}	--	1
Karst limestone	10^{-4}	--	1

Source: Adapted from Freeze and Cherry 1979.

Table 3-10. Representative Values for Saturated Moisture Contents and Field Capacities of Various Soil Types

		Saturated moisture content (θ_s)[a]		Field capacity (cm^3/cm^3)[b]	
	Number of soils	Mean	± 1 Standard deviation	Mean	± 1 Standard deviation
Sand	762	0.437	0.347 - 0.500	0.091	0.018 - 0.164
Loamy sand	338	0.437	0.368 - 0.506	0.125	0.060 - 0.190
Sandy loam	666	0.453	0.351 - 0.555	0.207	0.126 - 0.288
Loam	383	0.463	0.375 - 0.551	0.270	0.195 - 0.345
Silt loam	1,206	0.501	0.420 - 0.582	0.330	0.258 - 0.402
Sandy clay loam	498	0.398	0.332 - 0.464	0.255	0.186 - 0.324
Clay loam	366	0.464	0.409 - 0.519	0.318	0.250 - 0.386
Silty clay loam	689	0.471	0.418 - 0.524	0.366	0.304 - 0.428
Sandy clay	45	0.430	0.370 - 0.490	0.339	0.245 - 0.433
Silty clay	127	0.479	0.425 - 0.533	0.387	0.332 - 0.442
Clay	291	0.475	0.427 - 0.523	0.396	0.326 - 0.466

[a]From total soil porosity measurements compiled by Rawls et al. (1982) from numerous sources.
[b]Water retained at -0.33 bar tension; values predicted based on compiled soil property measurements.

Source: Rawls et al. 1982.

$$\Theta = (\Theta_s)^* (q/K_s)^{1/(2b+3))} \quad (3\text{-}13)$$

where

- Θ = volumetric water content in the unsaturated zone, (volume/volume or unitless).
- Θ_s = volumetric water content of soil under saturated conditions, (volume/volume or unitless).
- q = percolation rate (assumed to be equal to the unsaturated hydraulic conductivity term in original Clapp and Hornberger equation), (depth per unit time).
- K_s = saturated hydraulic conductivity, (depth per unit time).
- b = soil-specific exponential parameter, (unitless).

Representative values of "b" and the term "1/(2b+3)" are listed in Table 3-11.

Table 3-11. Representative Values of Hydraulic Parameters (Standard Deviation in Parentheses)

Soil texture	No. of soils[a]	b[b]		$\frac{1}{2b+3}$	Θ_s[c]	
Sand	13	4.05	(1.78)	0.090	0.395	(0.056)
Loamy sand	30	4.38	(1.47)	0.085	0.410	(0.068)
Sandy loam	204	4.90	(1.75)	0.080	0.435	(0.086)
Silt loam	384	5.30	(1.87)	0.074	0.485	(0.059)
Loam	125	5.39	(1.87))	0.073	0.451	(0.078)
Sandy clay loam	80	7.12	(2.43)	0.058	0.420	(0.059)
Silt clay loam	147	7.75	(2.77)	0.054	0.477	(0.057)
Clay loam	262	8.52	(3.44)	0.050	0.476	(0.053)
Sandy clay	19	10.40	(1.84)	0.042	0.426	(0.057)
Silt clay	441	10.40	(4.45)	0.042	0.492	(0.064)
Clay	140	11.40	(3.70)	0.039	0.482	(0.050)

[a]Number of individual soil samples included in data compiled by Clapp and Hornberger (1978).
[b]Empirical parameter relating soil matric potential and moisture content; shown to be strongly dependent on soil texture.
[c]Volumetric soil moisture content (volume of water per volume of soil).
Source: Adapted from Clapp and Hornberger 1978.

The saturated volumetric water content (Θ_s), saturated hydraulic conductivity (K_s), and the exponential function (b) are all related to soil properties. The most reliable values for these parameters are empirical values (if available) measured during site investigation. Where empirical values are unavailable, values in Tables 3-10 through 3-11 provide guides for the rough estimation of Θ_s, K_s, and the term 1/2b+3 . Representative values from two different sources are presented for K_s (Tables 3-8 and 3-9) and Θ_s (Tables 3-10 and 3-11), in order to demonstrate the variability in estimates for these values.

Note that the value Θ cannot exceed Θ_s, the saturated soil moisture content. When Θ calculated by Equation 3-13 equals or exceeds Θs, it must be assumed that saturated conditions exist. In such cases, use Equations 3-9 and 3-10.

Similarly, the minimum value for Θ that is applicable to Equation 3-13 is the field capacity of the soil. This value represents the volumetric moisture content remaining in the soil following complete gravity drainage and is the moisture content below which downward flow of water due to gravity through unsaturated soil ceases. Field capacity is a function of soil type; the most reliable values are those measured empirically. Where measured values are not available, default values can be taken from Table 3-10. Wherever Equation 3-13 results in a value for Θ that is less than the specific retention of the soil, it should be assumed that no downward movement of moisture (and dissolved contaminant) occurred for the associated time increment, and that V_{pw} is equal to zero.

Note that the percolation rate (q) cannot exceed the saturated hydraulic conductivity (K_s) for the site soil. Whenever $q \geq K_s$ (and therefore Θ as calculated by Equation 3-13 $\geq \Theta_s$) for the duration of the study period, it must be assumed that saturated conditions exist and that saturated flow prevails. Equations 3-9 and 3-10 in the preceding subsection provide a means of estimating saturated flow velocities.

The following equation provides an estimate of the term q (Enfield et al. 1982):

$$q = HL + P_r - ET - Q_r \quad (3\text{-}14)$$

where

- HL = hydraulic loading from manmade sources, (depth per unit time)
- P_r = precipitation, (depth per unit time)
- ET = evapotranspiration, (depth per unit time)
- Q_r = runoff, (depth per unit time).

Records of estimated percolation rates for the site locality during the time period in question (or annual average percolation rate estimates) are often available from local climate or soil authorities, including regional U.S. Geological Survey (USGS) and U.S. Soil Conservation Service offices.

An estimation procedure can be used to evaluate percolation rates (q) at sites where the sources listed above cannot provide them directly. This estimation procedure requires data for precipitation, evaporation, and runoff rates. In addition to the above two sources,

Table 3-12. Suggested Value for C_{et} Relating Evaporation from a US Class A Pan to Evapotranspiration from 8 to 15-cm Tall, Well-Watered Grass Turf

	Pan surrounded by a short green crop				Pan surrounded by a dry surface ground			
		Average regional relative humidity, %*				Average regional relative humidity, %*		
Wind	Upwind fetch of crop (m from pan)	20-40	40-70	>70	Upwind fetch of dry fallow (m from pan)	20-40	40-70	>70
	0	0.55	0.65	0.75	0	0.7	0.8	0.85
Light <170 km/day	10	0.65	0.75	0.85	10	0.6	0.7	0.8
	100	0.7	0.8	0.85	100	0.55	0.65	0.75
	1000	0.7	0.85	0.85	1000	0.5	0.6	0.7
	0	0.5	0.6	0.65	0	0.65	0.75	0.8
Moderate 170-425 km/day	10	0.6	0.7	0.75	10	0.55	0.65	0.7
	100	0.65	0.75	0.8	100	0.5	0.6	0.65
	1000	0.7	0.8	0.8	1000	0.45	0.55	0.6
	0	0.45	0.5	0.6	0	0.6	0.65	0.7
Strong 425-700 km/day	10	0.55	0.6	0.65	10	0.5	0.55	0.65
	100	0.6	0.65	0.7	100	0.45	0.5	0.6
	1000	0.65	0.7	0.75	1000	0.4	0.45	0.55
	0	0.4	0.45	0.5	0	0.5	0.6	0.65
Very strong >700 km/day	10	0.45	0.55	0.6	10	0.45	0.5	0.55
	100	0.5	0.6	0.65	100	0.4	0.45	0.5
	1000	0.55	0.6	0.65	1000	0.3	0.4	0.45

*Mean of maximum and minimum relative humidities.
Source: Jensen 1973, as presented by Enfield et al. 1982.

the National Weather Service, Forest Service offices, National Oceanic and Atmospheric Administration (NOAA) gauging stations, or other first order weather stations (e.g., at local airports) are possible sources for these three types of data.

The average precipitation rate per unit time (P_r) for the study period can be obtained from various local weather authorities such as those listed above.

ET is estimated by using measured Class A pan evaporation rates (a measure of local evaporation rates under standardized conditions, available from the nearest NOAA gauging station) in the equation:

$$ET = EVAP \times C_{et} \times C_{veg} \qquad (3\text{-}15)$$

where

EVAP = region-specific or site-specific measured evaporation rates, (depth per unit time).

C_{et} = correction factor for converting measured pan evaporation rates to evapotranspiration rates from turf grass, (unitless).

C_{veg} = correction factor for converting evapotranspiration from turf grass to evapotranspiration from other vegetative cover types, (unitless).

Values for C_{et} are taken from Table 3-12, which requires climatological and pan descriptive information.

The term C_{veg} is available mainly for agricultural crops (Table 3-13), and varies with the thickness, depth, and characteristics of vegetative cover. Typical values are 0.87 for shorter broadleaf plants (alfalfa) to 0.6 for taller broadleaf plants (potatoes, sugar beets) and 0.6 for taller grains and grasses. Where crop-specific data are unavailable, a conservative default value for this term is the smallest reasonable value, or 0.6.

Q_r, or the average runoff over the study period, is estimated by the method presented in Section 2.4 of this manual. A more reliable value for this term can be obtained from local USGS gauging stations. For relatively level sites, a reasonable conservative default value for the purposes of this estimation procedure is that $Q_r = 0$, where site-specific data are unavailable or cannot be estimated.

Table 3-13. Crop Coefficients for Estimating Evapotranspiration

Crop	Period	Coefficient (C_{Veg})
Alfalfa	April 1 - October 10	0.87
Potatoes	May 10 - September 15	0.65
Small grains	April 1 - July 20	0.6
Sugar beets	April 10 - October 15	0.6

Source: Jensen 1973, as presented by Enfield et al. 1982.

The above method for predicting the velocity of water migrating through the vadose zone is the best approximation available; however, real world non-homogeneities, such as root holes and macropores, can result in faster velocities than predicted. The analyst is not expected to correct for this, yet it is important to be aware of the limitations of the method.

3.5.2.3 Corrections for Viscosity and Density

When the movement of liquids other than water is calculated, the saturated and the unsaturated hydraulic conductivity must be corrected for the density and viscosity of the non-water liquid. The equation for this correction is as follows:

$$K_c = K_w \cdot (\text{density of chemical/density of water}) \cdot (\text{viscosity of water/viscosity of chemical}) \quad (3\text{-}16)$$

where

K_w = hydraulic conductivity of water (Darcy's coefficient), (saturated or unsaturated)

K_c = hydraulic conductivity of chemical, (saturated or unsaturated).

When the migration velocity through the vadose zone is calculated, density and viscosity should be corrected with the above equation. For horizontal flow below the water table, density and viscosity should be factored in when the hydraulic gradient is the slope of the chemical plume. In many cases, one can assume that the thickness of the concentrated chemical plume is relatively constant. For such situations, the slope of the concentrated chemical is zero and the analyst should not correct for the density. The slope (hydraulic gradient) is that of water, and the Darcy coefficient reflects the density of water. However, the viscosity of the chemical is the viscosity of the flowing fluid of concern, and the analyst should correct for the viscosity.

3.5.2.4 Retardation Effects

Hydrophobic or cationic contaminants that are migrating as a dilute solute are subject to retardation effects. Concentrated plumes are not subject to this phenomenon. Contaminant migration as a dilute solute in complex leachates containing organic constituents will show some retardation, although not as much as in pure ground water.

When a hydrophobic contaminant flowing in a dilute plume flows past a soil particle that contains organic carbon, the contaminant partitions between the polar solvent (water) and the solid organic carbon. When the concentration in the water is high and the concentration on the soil particle low, the net migration is from the water to the soil. When the reverse occurs and the concentration in the water is low and the concentration on the soil particle is high, the net migration is from the soil particle to the water. When the water and soil concentrations are in equilibrium, there is no net migration. However, the flux from the soil to the water and the flux from the water to the soil are not zero; rather, they are positive fluxes that are equal and are in opposite directions. When the partitioning is between concentrated chemical and soil particles, the contaminant does not prefer the solid "solvent" effects of the organic carbon in the soil to the organic liquid solvent effects of the concentrated chemical plume. Hence, hydrophobic contaminants partition out of polar solvents (water) but not out of hydrophobic solvents, and thus, retardation effects are modeled for dilute plumes only.

Retardation can be modeled for complex leachates, but the methods are not presented in this report. The reader is referred to Nkedi-Kizza et al. 1985, Rao et al. 1985, and Woodburn et al. 1986, for guidance on performing these calculations.

The retardation protocol is based on the assumption that adsorption of hydrophobic contaminants is due to sorption to organic carbon in the soil. Basing the adsorption coefficients on soil organic carbon rather than total mass eliminates much, but not all, of the variation in sorption coefficients between different soils. The remaining variation may be due to other characteristics such as surface area of soil particles per mass of soil (function of particle size). Numerous studies of the correlation of K_d with various soil variables have found that the organic carbon content usually gives the most significant correlation. Furthermore, this correlation often extends over a wide range of organic carbon content -- from 0.1 percent to nearly 20 percent of the soil in some cases (Lyman et al. 1982).

This protocol estimates hydrophobic retardation based on soil organic carbon, but it should not be taken to imply that hydrophobic contaminants will not adsorb on minerals free of organic matter. Some adsorption will always take place, and it may be significant under certain conditions, such as clay soils (high surface area per mass of soil) with very low organic carbon content (no appreciable sorption to nonexistent organic carbon). Unfortunately, methods

for estimating adsorption coefficients under these conditions are not currently available (Lyman et al. 1982). The protocol discussed in this report relies on the percent of organic carbon content of the soil.

To simplify modeling, equilibrium conditions are modeled as the contaminant velocity being a fraction of the ground-water velocity. If the analyst thinks of the time an individual portion of the contaminant mass is in the water as the time it has ground-water velocity, and the time the contaminant is on the soil particles as the time the contaminant does not have a velocity, the contaminant velocity is related to the ground-water velocity by the ratio of time on soil particles to time in the water. The ratio of time in the water to time on the soil particles is the same ratio as the concentration ratio at equilibrium.

In complex leachates containing organics, the time a hydrophobic contaminant spends on the solid carbon is reduced because the ratio of the contaminant's solubility in the fluid to its solubility on soil carbon is increased. The hydrophobic contaminant partitions between the organics in the flowing fluid and the organics that are solid.

The same logic applies to cation retardation, and the contaminant velocity for cations is also modeled as fraction of ground-water velocity.

The equation used to calculate the retardation is as follows (Kent et al. 1985):

$$R_d = 1 + (\beta * K_d)/p_t \qquad (3\text{-}17)$$

where

R_d = retardation factor, (unitless).
β = bulk density, (g/ml).
p_t = total porosity, (unitless).
K_d = distribution factor for sorption on aquifer medium (from sorption isotherm column studies, or from regression equation based on the octanol/water partition coefficient, (in ml/g).

The use of the retardation factor is described in the following equation (Kent et al. 1985):

$$R_d = v_{pw}/v_d \qquad (3\text{-}18)$$

where

R_d = retardation factor, (unitless).
v_{pw} = velocity of ground water, (same units as V_c' length/time).
v_d = velocity of contaminant, (same units as V_{gw}' length/time).

The term K_d is based on sorption isotherm column studies. While this is the more precise approach, the analyst will typically have to work with estimated parameters. For hydrophobic contaminants, the term K_d can be estimated from the term K_{oc} (Lyman et al. 1982):

$$K_{oc} = K_d/f_{oc} \qquad (3\text{-}19)$$

where

K_{oc} = partition coefficient for organic carbon, (ml/g).
K_d = distribution factor for soil, (ml/g).
f_{oc} = fraction of organic carbon in the soil.

The term "fraction of organic carbon" (f_{oc}) is precise when taken from empirical measurements of the soil in the study area. For cases where this is not possible, estimates can be made. For the vadose zone velocity, a value of f_{oc} from Rawls (1986) provides a good estimate. Rawls' work focused on soils near the surface, the area of interest to agriculture. For saturated zone velocity, the analyst has two choices. If the subsoil came from igneous or metamorphic rock, the f_{oc} decreases with depth. The actual value may be quite low; however, the model to predict retardation is only useful down to 0.1 percent. For this situation, the analyst should use 0.1 percent for the f_{oc}. If the subsoil came from sedimentary rock, the f_{oc} distribution may be similar to the distribution for agricultural soils done by Rawls. The variation of f_{oc} with depth may be relatively constant. The carbon was at the surface at one time, and has been buried over geological time. Hence, the analyst should use a value of f_{oc} from the Rawls (1986) distribution for the saturated zone velocity determination (Trask and Patnode 1942). Soil/water partition coefficients have been developed for many contaminants of importance (Callahan et al. 1979 and Mabey et al. 1982).

If K_{oc} is not known, it can be estimated from regression equations that relate K_{oc} to K_{ow} (octanol/water partition coefficient). There are six regression equations that relate K_{oc} to K_{ow}. The equation that was based on a chemical class closest to the subject contaminant should be used. If the contaminant does not fit into a specific class, the first regression equation should be used because it was based on the largest sample. The regression equations are as follows (Lyman et al. 1982):

$$\text{Log } K_{oc} = 0.544 \log K_{ow} + 1.377 \qquad (3\text{-}20)$$

based on a wide variety of contaminants, mostly pesticides

or

$$\log K_{oc} = 0.937 \log K_{ow} - 0.006 \quad (3\text{-}21)$$

based on aromatics, polynuclear aromatics, triazines and dinitroaniline herbicides

or

$$\log K_{oc} = 1.00 \log K_{ow} - 0.21 \quad (3\text{-}22)$$

based on mostly aromatic or polynuclear aromatics

or

$$\log K_{oc} = 0.94 \log K_{ow} + 0.02 \quad (3\text{-}23)$$

based on s-triazines and dinitroaniline herbicides

or

$$\log K_{oc} = 1.029 \log K_{ow} - 0.18 \quad (3\text{-}24)$$

based on a variety of insecticides, herbicides, and fungicides

or

$$\log K_{oc} = 0.524 \log K_{ow} + 0.855 \quad (3\text{-}25)$$

based on substituted phenylureas and alkyl-N-phenylcarbamates.

The retardation effects are computed from the octanol/water partition coefficient (K_{ow}), which relates the concentration in polar solvent (water) to the concentration in hydrophobic solvent (octanol simulating the soil organic carbon). If the contaminated plume has a large concentration of organic chemicals dissolved in the ground water, the actual partitioning will be from a solvent/organic chemical system. This will raise the concentration in the fluid and lower the concentration on the soil organic carbon. This shift in partitioning will lower R_d, (i.e., the contaminant will migrate at a speed closer to that of ground water). Much of the solubility of extremely hydrophobic contaminants in the water of an octanol/water partition coefficient test is due to dissolution in the octanol that is dissolved in the water rather than dissolution into water. This effect depends on the degree to which the water is not pure water; for most low-level contamination situations, this effect can be ignored. This manual does not present equations for calculating a numerical correction for this effect. The analyst should be aware of the general influence of this effect, but not model the precise numerical difference. For dilute plumes, the analyst should model full retardation; for concentrated plumes, the analyst should model no retardation.

3.5.2.5 Contaminant Velocity

The velocity of concern is the actual contaminant velocity. The determination of ground-water velocity discussed earlier is done to provide a foundation for calculating the contaminant velocity. The particular method used for determination of the contaminant velocity is dependent on the type of ground-water transport the chemical undergoes. Thus, the first step in calculating the velocity is classifying the subject contaminants as to migration class.

Once the molecular identity of the contaminant is known, three determining parameters can be taken from literature:

1. Physical state at room temperature (i.e., is it a solid or a liquid?)
2. Hydrophobicity (i.e., is it hydrophilic or hydrophobic?)
3. Density (i.e., is it less dense than water?, Is its density near that of water?, Or is it more dense than water?)

The five migration classes are as follows:

Migration class #	Vadose zone transport	Saturated zone transport
A)	Solid/carried by precipitation	Solute transport
B)	Hydrophilic liquid/ waste percolation	Solute transport
C)	Hydrophobic liquid/ waste percolation	Low density/ floater transport
D)	Hydrophobic liquid/ waste percolation	Medium density/ buoyant transport
E)	Hydrophobic liquid/ waste percolation	High density/ sinker transport

Although the specific chemical will migrate according to the above classes, it is important to note that the concentrated plumes will also have a dilute plume near them. For mass flux considerations, the concentrated plume will dominate.

(1) Migration Class #A: Solid Material

Solid material will dissolve into percolating precipitation and migrate as a solute. Precipitation provides the hydraulic loading that drives the rate of release. The plume exists as a single plume (for single chemical contaminant) that has a single average velocity. Unretarded contaminants move with the ground water, and hence, the ground-water velocity is the contaminant velocity. Retarded contaminants move with a velocity that is slower than ground-water velocity, and therefore the contaminant velocity is based on the ground-water velocity adjusted for retardation. Typically, the velocity is a fraction of the ground-water velocity.

(2) Migration Class #B: Hydrophilic Liquids

Liquids will directly percolate into the soil (i.e., without waiting for precipitation to cause leaching). The

hydraulic loading is due to the combination of chemicals' hydraulic loading and that due to precipitation. The velocity of transport through the vadose zone must be calculated with corrections for the density and viscosity of the contaminant. The plume exists as a single plume (for a single chemical contaminant) that can be considered to have a single average velocity. Unretarded contaminants move with the ground water, and hence, the ground-water velocity is the contaminant velocity. This is only exact after the plume has mixed with the ground-water to the point that its density and viscosity are similar to those of water. When the plume first reaches the water table, it has not mixed with very much water, and its density and viscosity differences suggest calculating a contaminant velocity that is different from the ground-water velocity. Since the velocity difference varies gradually from the source to the point downgradient where it is well mixed, this calculation is complex. Therefore, the analyst should calculate as if the ground-water velocity represented the contaminant velocity for the length of the plume. The analyst should be aware of the limitations of this method. Retarded (cationic) contaminants move with a velocity that is slower than ground-water velocity. In this case, contaminant velocity is based on the ground-water velocity adjusted for retardation, and is a fraction of the ground-water velocity.

(3) Migration Class #C: Hydrophobic Liquids/Low Density

Once hydrophobic liquids reach the water table, they form two distinct plumes (for a single chemical contaminant), with each having its own average velocity. The concentrated plume will float on the surface of the water table and move in the same direction as the ground-water flow. Its velocity is a function of the contaminant's viscosity. If mounding is significant, the density must also be considered. The dilute plume is formed by small amounts of the chemical dissolving in water as limited by the hydrophobic chemical's solubility. This plume will be found below the concentrated plume, with the highest concentration near the concentrated plume. From the point where the contamination leaves the concentrated plume to form the dilute plume, the dilute plume will move with the ground-water flow (at a retarded velocity). The concentrated plume will have a single average velocity, and it will start at the location of the source. The dilute plume will have a single average velocity, but its starting point can be from the location of the source, or it can form from the concentrated plume anywhere along the length of the concentrated plume.

Retarded contaminants in the dilute plume move with a velocity that is slower than ground-water velocity. Thus, contaminant velocity, based on the ground-water velocity adjusted for retardation, is typically a fraction of the ground-water velocity. Contaminants in the concentrated plume do not move with the ground-water velocity; their velocity must be determined by considering the effect of the hydrophobic contaminant's viscosity. The concentrated plume does not exhibit retardation effects. If mounding is significant, the analyst also must factor in the density.

(4) Migration Class #D: Hydrophobic Liquids/Medium Density

This class of compounds migrates similarly to Class #3, except that the concentrated plume will not float or sink, but will have more or less neutral buoyancy. It will move in the direction of ground-water flow, but its migration velocity will be a function of its viscosity. Again, the dilute plume will surround the concentrated plume, forming a transition zone between the uncontaminated water and the concentrated plume body. From the point where the contaminant leaves the concentrated plume to form the dilute plume, the dilute plume will move with the ground-water flow (at a retarded velocity). The concentrated plume will have a single average velocity, and it will start at the location of the source, or it can form from the concentrated plume anywhere along the length of the concentrated plume.

Retarded contaminants in the dilute plume move with a velocity that is slower than ground-water velocity. Thus, the contaminant velocity, based on the ground-water velocity adjusted for retardation, is a fraction of the ground-water velocity. Contaminants in the concentrated plume do not move with the ground-water velocity; their velocity must be determined by considering the effect of the hydrophobic contaminant's viscosity. The concentrated plume does not flow with retardation effect.

(5) Migration Class #E: Hydrophobic Liquids/High Density

As with low and medium density hydrophobics, once a high density plume reaches the water table, it forms two distinct plumes (for a single chemical contaminant) with each having its own average velocity. The concentrated plume will sink to the bottom of the aquifer. Its velocity is a function of the contaminant's viscosity. If mounding on the aquitard is significant, the density must also be considered. The dilute plume will be above the concentrated plume, with the highest concentration near the concentrated plume and the lowest concentration at the farthest distances from the concentrated plume. The concentrated plume will have a single average velocity and will start at the location of the source. The dilute plume will have a single average velocity, but its starting point can be from the location of the source, or it can form from the concentrated plume anywhere along the length of the concentrated plume.

Retarded contaminants in the dilute plume move with a velocity that is slower than ground-water velocity. Thus, the contaminant velocity, based on the ground-water velocity adjusted for retardation, is a fraction of the ground-water velocity. Contaminants in the concentrated plume do not move with the ground-water velocity; their velocity must be determined by considering the effect of the hydrophobic contaminant's viscosity. If the sinker mounds above the aquitard significantly, the density should be taken into consideration. The concentrated plume does not flow with retardation effects.

3.5.2.6 Nomograph Technique

The following nomograph is based on a solution to solute transport in an aquifer from a point source that extends throughout the thickness of the aquifer. Contaminant transport from the source includes advective flow with the ground water and longitudinal and transverse dispersion (see Wilson and Miller 1978). The nomograph is taken from Kent et al. (1985); the analyst is referred to this source document for further discussion of the use of the nomograph and its limitations.

The nomograph, which is a one-dimension model (results restricted to a line, dispersion is two-dimensional), is intended as a rapid means to obtain an approximate solution. Scale factors are used to translate Wilson and Miller (1978) to nomograph form. Dilution/dispersive mixing and retardation parameters are included in the solution.

Three scale factors that must be calculated before using the nomograph are:

$$X_D = \frac{Dx}{v} \qquad (3\text{-}26)$$

$$T_D = \frac{Rd\ Dx}{V^2} \qquad (3\text{-}27)$$

$$Q_D = P_e m \sqrt{Dx\ Dy} \qquad (3\text{-}28)$$

Two of the three ratios are computed directly, and the third is found using the nomograph (Figure 3-8). The procedure for calculating the scaling factors and using the nomograph is presented as follows:

(1) Scale Factor Development

This nomograph models the same variety of conditions that the Wilson and Miller model (from which it was derived) does, yet it does it with only one graph. This was achieved by scaling the parameters to make them dimensionless. Distance X is made dimensionless by dividing by the distance scaling factor (X_D, the characteristic dispersion length). The mass flux ($Q * C_o$) is made dimensionless by dividing by the mass flux scaling factor (Q_D). And time (T) is made dimensionless by dividing by the time scaling factor (T_D). Obtain X_D using the following:

$$X_D = \frac{Dx}{v} \qquad (3\text{-}29)$$

where variables are defined as in Figure 3-8, Definition of Terms.

Calculate T_D using

$$T_D = \frac{R_d * D_x}{V^2} \qquad (3\text{-}30)$$

where

V	=	$(K^s * i)/P_e$.
R_d	=	$1 + \beta * K_d/P_t$.
T_d, D_x	=	defined in Figure 3-8, Definition of Terms,

and where

$$K_d = f_{oc} * K_{oc}.$$

Calculate Q_D using:

$$Q_D = P_e * m * (D_x * D_y)^{1/2} \qquad (3\text{-}31)$$

where variables are defined as in Figure 3-8, Definition of Terms.

(2) Application of Scale Factors

Use the three scale factors and the nomograph (Figure 3-8) to calculate the concentration at time T and distance X.

(a) Find T/T_d curve desired.

(b) Find X/X_d on the x-axis.

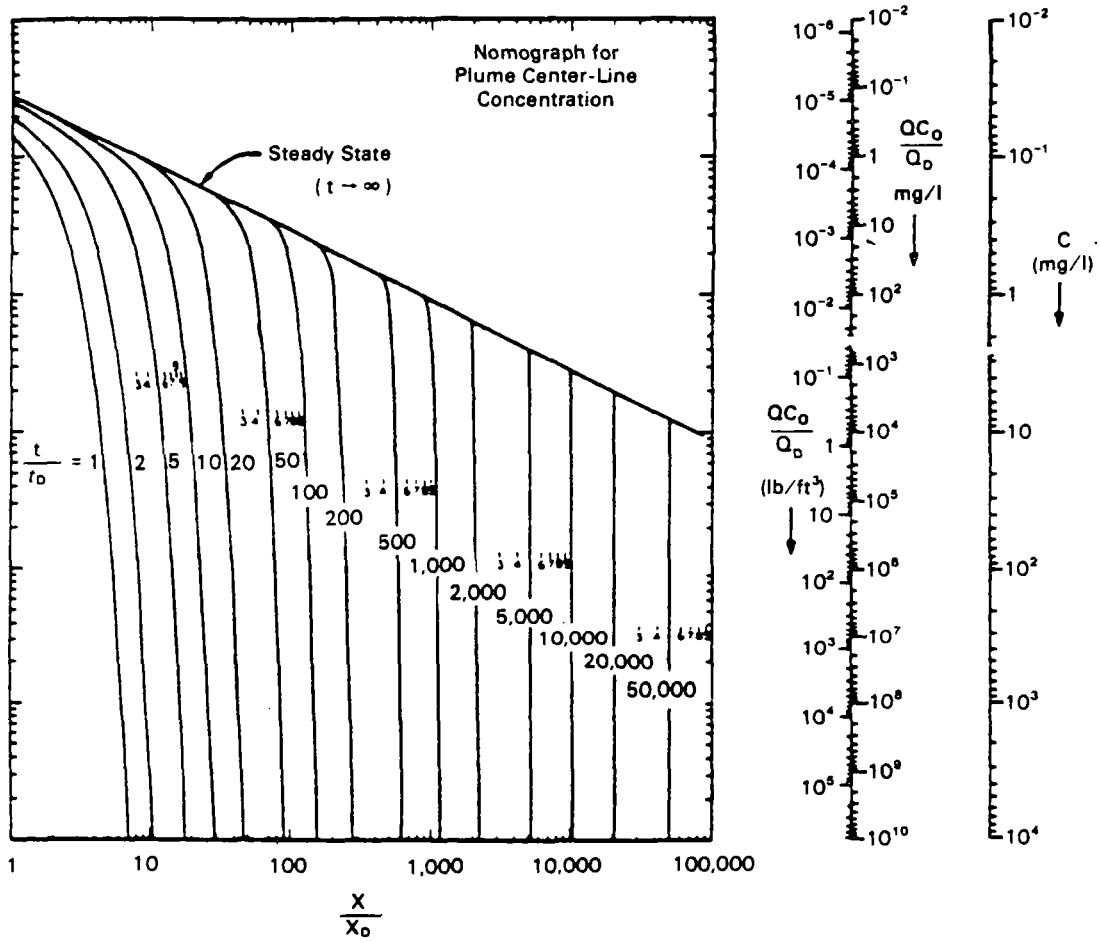
(c) Plot the point of intersection of the T/T_d curve and X/X_d.

(d) Use this point and the point on the $Q * C_o/Q_d$ line to draw a straight line. Where this line intersects the concentration line, the concentration at distance X and time T is indicated.

3.5.2.7 Extent of Plume

As discussed earlier, a large volume of contaminated ground water can result from a small volume of chemical release. For example, a 10-gallon spill of solvent can contaminate a billion gallons of ground water to 10 ppb. Similarly, a 5000-gallon tanker truck can contaminate 500 billion gallons of ground water to 10 ppb. The analyst must be aware of the relationship between volume of contaminant released and volume of contaminated ground water. The

Figure 3-8. Nomograph for solutions of time, distance, and concentration for any point along the principal direction of groundwater flow.



Source: Kent et al. (1985)

Figure 3-8. (Continued)

Definition of Terms

Primary Variables : ***Units***

C	=	concentration of leachate at a specific time and distance.	(M/L^3)
X	=	distance from source where concentration of leachate is computed. distance is measured in direction of ground-water flow (perpendicular to gradient).	(L)
y	=	transverse distance measured from the centerline of ground-water flow (assumed to be zero in the nomograph).	(L)
t	=	sample time from beginning of leachate source flow.	(T)

Aquifer Parameters :

m	=	effective aquifer thickness or zone of mixing.	(L)
P_e	=	effective porosity of aquifer or zone of mixing.	(Dimensionless)
v	=	velocity of ground-water flow within voids, estimated directly from:	

$$v = \frac{Ki}{P_e}$$

where

K	=	coefficient of permeability or hydraulic conductivity of aquifer or zone of mixing.	
i	=	gradient of ground-water flow.	(Dimensionless)

Transport Parameters :

D_x	=	longitudinal dispersion coefficient (mixing rate) with respect to distance in x direction and time, estimated directly or from:	(L^2/T)

$$D_x = a_x v + D^*$$

where

a_x	=	longitudinal dispersivity.	(L)
D^*	=	molecular diffusion coefficient, which is assumed to be negligible for velocities typical of permeable aquifers. D^* may be the dominant process in aquitards where a_x V would be negible.	(L^2/T)

Figure 3-8. (Continued)

Definition of Terms

Units

D_y = Transverse dispersion coefficient (mixing rate) with respect to distance in the y direction and time, estimated directly or from: (L^2/T)

$$D_y = \alpha_y v + D^*$$

where

α_y = transverse dispersivity. (L)

or estimated as:

D_y = D_x divided by a ratio, which commonly ranges between 5 and 10 for medium to coarse sand aquifers.

R_d = Retardation factor estimated directly or from: (Dimensionless)

$$R_d = 1 + \frac{\beta b(K_d)}{P_t} \text{ (or) } R_d = \frac{v}{Vd}$$

where

βb	=	bulk density of aquifer medium.	(M/L^3)
P_t	=	total porosity.	(Dimensionless)
K_d	=	distribution factor for sorption on aquifer medium (from sorption isotherm column studies)	(L^3/M)
v	=	velocity of ground water.	(L/T)
v_d	=	observed velocity of leachate for a given concentration and chemical species.	(L/T)
γ	=	coefficient for radioactive or biological decay. For no decay, the value of γ is one. (Assumed to be one in the nomograph.) Calculated from:	(Dimensionless)

$$\gamma = 1 + \frac{4Dx}{v^2}\lambda = 1 + \frac{4Dx \log(2)}{v^2 t_{1/2}}$$

where

$$\lambda = \text{decay constant} = \frac{\log(2)}{t_{1/2}}$$ (1/T)

$t_{1/2}$ = Half-life: time when half of the original mass remains. (T)

Figure 3-8. (Continued)

Definition of Terms

			Units
Source Rate of Leachate :			
QC_0	=	Mass flow rate:	(M/T)
		where	
Q	=	Volume flow rate estimated directly or from:	(L^3/T)

$$Q = Aq$$

where

A	=	area of source.	(L^2)
q	=	recharge rate.	(L/T)
C_0	=	Initial concentration	(M/L^3)

Intermediate Variables (used for nomograph only) :

X_D = A characteristic dispersion length or scale factor given by: (L)

$$X_D = \frac{D_x}{\gamma v}$$

T_D = A characteristic dispersion time or scale factor given by: (T)

$$T_D = \frac{R_d D_x}{\gamma v^2}$$

Q_D = A characteristic dilution-dispersion flow given by: (L^3/T)

$$Q_D = P_e\, m \sqrt{D_x D_y}$$

equation is a simple mass balance equation and is expressed as follows:

For liquid contaminants:

$$V_l * C_l = V_{gw} * C_{gw} \quad (3\text{-}32)$$

where

V_l = volume of liquid chemical released.
V_{gw} = volume of contaminated ground water.
C_l = average concentration of chemical contaminant in the released liquid.
C_{gw} = average concentration of contaminant in ground water.

Both volumes and concentrations should be in the same units.

For solid contaminants:

$$M_c * C_c = C_{gw} * V_{gw} \quad (3\text{-}33)$$

where

M_c = mass of solid waste, (in milligrams).
C_c = concentration expressed as mass fraction, fraction of contaminant in waste, (dimensionless).
C_{gw} = concentration of contaminant in ground water, (mg/liter).
V_{gw} = volume of contaminated ground water, (liters).

To convert the quantity of contaminated ground water to a volume of contaminated soil, the following equation is used:

$$(V_{gw} * 0.13368)/P_t = V_c \quad (3\text{-}34)$$

where

V_{gw} = volume of contaminated ground water, (in gallons).
P_t = total porosity, (dimensionless fraction).
Vc = volume of contaminated soil, (in cubic feet).

Or alternatively:

$$V_{gw}/P_t = V_c \quad (3\text{-}35)$$

where both volumes are in the same units.

3.5.2.8 Use of Monitoring Data

The analyst should take care when using monitoring data to assess the depth of contamination in order to calculate volume or mass in the plume. The difference between monitoring and pumping wells will affect the interpretation of the concentrations found in the wells. Monitoring wells are the more desirable, but since most existing wells will be pumping wells, monitoring wells will typically have to be installed. The cost associated with drilling monitoring wells most likely will cause the analyst to rely on existing pumping wells.

Monitoring wells extract a small quantity of water (a sample); this minimizes the well's influence on the flow of the ground-water. They do not induce a large vertical component in the ground-water flow, and thus they sample a horizontal slice of the aquifer. The concentration in a sample removed from a monitoring well represents a concentration at the depth of the well screen. Thus, monitoring wells at various depths can be used to assess the depth of contamination.

Pumping wells draw large quantities of water from an aquifer (a pumping well provides water). This causes a cone of depression to form on the water table and influences the flow direction above and beneath the well screen. Pumping wells induce vertical flow in the aquifer near the well. This vertical movement causes the concentration in the well to reflect the average concentration for a depth range that is substantially greater than the length of the well screen. Water will be drawn from above and below the well screen. The well water does not reflect the concentration of a particular depth, but rather reflects an average concentration from a range of depths. This makes an assessment of the depth of contamination difficult. However, it makes assessing the mass in the plume easier since the well draws a sample that represents the concentrations at a wide range of depths near the well screen depth.

3.5.2.9 VHS Model

In addition to the nomographic technique, the Office of Solid Waste (OSW) has developed a simplified model for its delisting program that relates leachate concentration to receptor well concentration 500 feet downgradient from the edge of a landfill. The approach is called the VHS model (Vertical and Horizontal Spread model). The only reduction in concentration provided by the VHS model is that due to vertical and horizontal dispersion (OSW plans to add hydrolysis and biodegration for organics). The approach involves back calculating from a health-based ground-water concentration at the exposed population location to an acceptable leachate concentration at the site. Wastes with leachate above this concentration must be managed as hazardous wastes. Those with leachate below this concentration can be managed in a municipal landfill or

nonhazardous industrial landfill (i.e., outside the hazardous waste system).

The only data the VHS model requires are the leachate concentration and the annual volume of wastes disposed of (constituent concentrations of toxicants are also required in order to ensure that they are present in sufficient mass to sustain leaching). The model calculates a different dilution factor depending on the annual volume of waste disposed of. For Superfund purposes, the total volume of waste at the site would be used as the "Annual Volume of Waste" term. A small volume of waste can rely on greater dilution, while a large volume of waste is assigned a smaller dilution potential. All other input parameters are fixed at reasonable worst-case values. By fixing the environmental parameters, the model assumes a generic environment that is consistent with OSW's requirements. For CERCLA purposes, the model is considered to be useful as a simplified analytical procedure, and use of the VHS model for site-specific, in-depth analysis is not recommended.

When using this model, one should keep its limitations in mind. The VHS model simulates soluble toxic constituents dissolving into percolating precipitation and moving with the ground water. It does not address solvent transport of organics (two-phase flow) or the percolation of organic fluids into the ground.

Critics of the VHS model have pointed out two weaknesses of the approach. The first point is that the model upon which the VHS model was based (the Domenico and Palciaukas model) does not relate leachate concentration to exposed population well concentration. This model relates the concentration in ground water immediately below the hazardous waste sites to the exposed population well concentration. When leachate enters ground water, it will be mixed with ground water. This contaminates ground water and at the same time dilutes the concentration of leachate. It is wrong to use the C_O term in the model as leachate concentration, because it represents the concentration in ground water at the vertical point where leachate enters. This concentration must be measured on a site-specific basis to make the use of the model consistent with the boundary conditions used in the derivation of the model. The model is derived from the following assumptions:

1. Steady-state concentrations are achieved under the conditions that the concentration C_O in ground water is maintained on a vertical plane of finite size.

2. No longitudinal dispersion occurs; dispersion only in the y and z directions is assumed.

3. Recharge or dilution mechanisms, other than ground-water flow and the above-mentioned dispersion, are ignored.

4. The contaminant velocity in ground water is known.

The second weakness is the method used to determine the cross-sectional area of the plume at the edge of the landfill. The depth of the plume is determined by the horizontal velocity of ground water and the vertical velocity of the contaminant. The model presumes that the vertical velocity of the contaminant in the vadose zone is also the vertical velocity of the contaminant in the saturated zone. In the vadose zone, the contaminants are under the influence of gravity; in the saturated zone, the vertical velocity is much smaller because the effect of gravity is canceled by the buoyancy forces. The VHS model assumes that the velocities are the same.

These two weaknesses were present in the VHS model at the time this document was written; subsequent revisions may address these problems.

3.5.3 In-Depth Methods and Models

Several references are available that provide detailed derivations and outline the application of more sophisticated equations for the analysis of contaminant migration in the saturated and unsaturated zones. The analyst is referred to the following documents: USEPA 1985j; Van Genuchten and Alves (1982), Walton (1984), and Javendel et al. (1984), USEPA (1986a), Geotrans (1986), and van der Heijde (1985 and 1987).

Tables 3-14, 3-15, and 3-16 provide information regarding several modeling procedures for the in-depth assessment of the ground-water fate of hazardous substances. Note that in order to provide the analyst with an indication of the large number of computer models that could be applied to analysis of contaminant fate in ground water, Table 3-15 (Features of Unsaturated Zone and Ground-Water Fate Models) provides data for 24 models in addition to the 11 for which more detailed information is provided in Tables 3-14 and 3-16. Two of the models addressed in these tables are part of GEMS: SESOIL and AT123D. The latter is described in greater detail below, because it is more versatile and is applicable to a wide range of fate analysis situations. Additionally, following that discussion further detail for certain of the models addressed in Tables 3-14, 3-15, and 3-16 is also provided.

AT123D (*Analytical Transient 1-, 2-, or 3-Dimensional Simulation Model*) is capable of simulating the transport and fate of hazardous material under 300 different user-selected situations (Yeh 1981). One of eight source configurations can be selected: a point source; line sources aligned in

Table 3-14. Resource Requirements and Information Sources : Unsaturated Zone and Ground-Water Fate Models

Model	Description	Resource requirements, comments	References, sources of documentation, software
Unsaturated zone			
Seasonal Soil Compartment Model (SESOIL)	• Long-term fate simulations • Accounts for numerous hydrologic, meteorologic characteristics of site • Accounts for numerous transfer, transformation processes: adsorption volatilization, degradation, biodegradation • Models organics, inorganics • Produces contaminant concentration distribution in unsaturated zone, quality of ground-water runoff • Handles up to three layers of soil types, permeabilities	• Integrated into GEMS (see Section 3.1) • Versatile, easy to use • FORTRAN program language; has been implemented on IBM 370, VAX 11/780	*Documentation:* Bonazountas and Wagner 1981 *Contact for access to GEMS system:* Mr. Loren Hall U.S. EPA, Exposure Evaluation Division Washington, D.C. (202) 382-3931
PRZM (Pesticide Root Zone Model)	• One-dimensional • Organic substances • Degradation is simulated • Provides pollutant velocity, distribution, and concentration data • Accommodates various release rates, schedules	• PC Based Model • Requires 256 K RAM minimum, 640K preferred, • Intel 8089 or 80287 math coprocessor • Has been field-verified with pesticides • FORTRAN program language	*Reference*: Carsel et al. 1984 *Information:* David Disney USEPA Environmental Research Laboratory Athens, Ga. 30613 (909) 546-3132
PESTAN	• One-dimensional • Organic substances • Degradation is simulated • Provides pollutant velocity, distribution, and concentration data • Accommodates various release rates, schedules	• Considered a screening model • Rapid evaluations • Inexpensive, easy to use; requires only hand-held calculator • Has been field-verified with pesticides	*Reference*: Enfield et al. 1982

(Continued)

Table 3-14. (Continued)

Model	Description	Resource requirements, comments	References, sources of documentation, software
Hydrologic evaluation of landfill performance (HELP) (as modified by Anderson-Nichols)	• One-dimensional • Models leaching from landfills to unsaturated soil beneath landfill • Has four options to handle modeling the solubilization of toxic constituents • Models organics/inorganics • Uses rainfall and waste solubility to model leachate concentrations leaving landfill	Four options allow modeling with available data	*Information:* Brian Bicknell Anderson-Nichols Palo Alto, Calif. 94303 (415) 493-1864
Saturated zone Random Walk Solute Transport Model (RWSTM) (a.k.a. TRANS) (requires PLASM for flow modeling)	• One- or two-dimensional • Time-variant release rates • Accommodates well-injected release • Incorporates dispersion, retardation • Handles nonconservative pollutants • Accounts for well pumping • Provides contaminant concentration at user-selected points	• Requires mathematical programming, hydrogeological knowledge on part of user • Has been field-validated	*Documentation:* Prickett et al. 1981
Coupled Fluid, Energy and Solute Transport (CFEST) Combined with UNSAT-ID	• Three-dimensional • Accommodates heterogeneous, anisotropic, multilayered soil configurations • Handles saline aquifers as well as fresh water • Transport mechanisms of dispersion, advection simulated • Sorption, degradation mechanisms not incorporated • Time-variant release and flow rates • Combination covers unsaturated and saturated zones	• Has been applied for arsenic and organic wastes	*Documentation:* Gupta et al. 1987

(Continued)

Table 3-14. (Continued)

Model	Description	Resource requirements, comments	References, sources of documentation, software
Sandia Waste Isolation Flow and Transport Model (SWIFT and SWIFT II)	• Three-dimensional • Transport processes of advection, dispersion simulated • Sorption, degradation processes accounted for • Appropriate for waste-injection, waste-isolation modeling • Code was based on SWIP Model	• Has been field-verified • Has associated user's guide in self-teaching format • FORTRAN program; has been implemented on various CDC systems including CDC 7600 • 1986 version has been released	*Documentation:* Reeves and Cranwell 1981; Finley and Reeves 1968 *Software:* National Energy Software Center Argonne National Laboratories Argonne, Ill. 60439 *Information:* Intera Environmental Consultants, Inc. 11999 Katy Freeway, Suite 610 Houston, Tex. 77079
Leachate Plume Migration Model (LPMM)	• Continuous source model • Dispersion is simulated • Degradation processes accounted for • Has been field verified • A simplistic model; results may not be as sophisticated as necessary for Level III work	• Can be used in nomographic, hand-held calculator, or computer form • Relatively easy to use	*References:* Kent et al. 1982
Analytical Transient One-, Two-, and Three-Dimensional Simulation Model (AT123D)	See Section 4.4.2 of text	• FORTRAN program applicable to wide range of computers • May require extensive setup time • Available through GEMS (see Section 4.1)	*Documentation:* Yeh 1981

(Continued)

Table 3-14. (Continued)

Model	Description	Resource requirements, comments	References, sources of documentation, software
Unsaturated and Saturated Zones			
Finite-Element Model of Waste (FEMWASTE) and Finite Element Model of Water Flow (FEMWATER)	• Two-dimensional • Interzone transfer is modeled • Incorporates convection, dispersion • Simulates degradation of nonconservative substances • Adsorption is accounted for • Capable of modeling layered, heterogeneous soil zones • FEMWATER is a model for ground-water flow, while FEMWASTE simulates the transport/fate of contaminants	• Has been implemented on IBM 360 • May require background in hydrogeology, differential equations, programming • Field-verified	*Documentation:* Yeh and Ward 1981 *Information:* Dr. George T. Yeh Oak Ridge National Laboratory Environmental Science Division P.O. Box X Oak Ridge, Tenn. 37830 (615) 574-7285
Solute Transport and Dispersion Model	• Two-dimensional • Conservative substances (no decay simulation) • Heterogeneous soil conditions accounted for • Pumping or recharging well effects modeled • Thickness of saturated zone may vary	• Field Verified • Relatively inexpensive, easy to use	*Documentation:* Kowikow and Bredehaeft 1974

Sources: USEPA 1982b; Brown et al. 1983; Kufs et al. 1983; Versar 1983.

Table 3-15. Features of Unsaturated Zone and Ground-Water Fate Models

Model	SOIL/ROCK CHARACTERISTICS										FLUID CONDITIONS							FLOW CONDITIONS						REFERENCE CITATION
	CONFINED AQUIFERS	WATERTABLE AQUITARDS	MULTIPLE AQUIFERS	HETEROGENEOUS AQUIFERS	ANISOTROPIC	FRACTURED	SINGLE SOILS LAYER	LAYERED SOILS	MATRIX DEFORMATION	SINGLE FLUID	MULTIPLE FLUIDS	MISCIBLE	IMMISCIBLE	FRESH WATER	SALT WATER	N.a.p.l.*	GAS/AIR	VARYING DENSITY	SATURATED	UNSATURATED	STEADY STATE	TRANSIENT		
AT123D	●										●									●		●		Yeh 1981
LPMM	●										●									●		●		Kent et al. 1986
ONE-D	●										●									●		●		van Genuchten and Alves 1982
Plume (3D)	●										●									●		●		Codell et al. 1982
Reseq	●										●									●		●	●	Javendel et al. 1984
SLM	●		●					●			●									●	●	●		Huyakorn et al. 1987
VHS	●										●									●		●		Domenico and Palciauskas 1982
RW-Analyt.	●										●									●		●	●	van der Heijde and Grinivasan 1986
Beaver Bolt	●		●		●	●					●		●	●	●	●			●	●		●	●	Bear and Verruijt 1987
Kinzelbach	●		●		●	●					●									●		●	●	Kinzelbach 1986
Walton 3S	●										●									●		●		Walton 1989
Solute	●										●									●		●		Beijin 1986
Femtran			●		●	●		●	●		●									●	●	●	●	Martinez 1986
Femwater/Femwaste	●	●	●	●	●	●		●	●		●									●	●	●	●	Yeh 1987, Yeh, and Ward 1981
Porflo	●	●		●	●	●				●	●								●	●	●	●	●	Runchal et al. 1986
GS2/GS3	●	●	●	●	●	●		●	●		●									●	●	●	●	Davis and Bagel 1986
PRZM								●	●		●										●	●	●	Carsel et al. 1984
SESOIL								●			●										●	●	●	Bonazountas and Wagner 1984
SUMATRA-1								●	●		●									●	●	●	●	van Genuchten 1978
SUTRA	●	●	●	●	●	●		●	●		●								●	●	●	●	●	Voss 1984
TRIPM	●	●	●	●	●	●		●	●		●									●	●	●	●	Gureghian 1983
CFEST	●	●	●	●	●	●					●									●		●	●	Gupta et al. 1987
FEWA/FEMA	●		●		●	●					●									●		●	●	Yeh and Huff 1985
HST3D	●	●	●		●	●					●								●	●		●	●	Kipp 1987
MOC(USGS 2-D)	●				●	●					●									●		●	●	Konikow and Bedekoeft 1978
MOC DENSE	●				●	●						●		●	●	●			●	●		●	●	Sanford and Konikow 1985
MOC NRC	●		●		●	●					●									●		●	●	Tracy 1982
RWSTM	●		●		●	●					●									●		●	●	Prickett et al. 1981
SWENT	●	●		●	●	●					●								●	●		●	●	Intera 1983
SWIFT II	●	●	●	●	●	●	●				●								●	●		●	●	Reeves et al. 1986
TRACR 3D	●	●		●	●	●	●			●	●	●	●	●	●			●		●	●	●	●	Travis 1984
TRAFRAP/WT	●		●		●	●	●				●									●		●	●	Huyakorn et al. 1987
BIOPLUME-II	●		●		●	●					●									●		●	●	Rifai et al. 1987
PESTAN								●			●										●	●	●	Enfield et al. 1982
HELP								●			●										●	●	●	See table 3-14

*NON-AQUEOUS PHASE LIQUIDS 1) FOR UNSATURATED ZONE ONLY.

Table 3-15. (Continued)

Model	GEOMETRY						TRANSPORT AND FATE PROCESSES											REFERENCE CITATION
	1-DIMENSIONAL (VERTICALLY AVERAGED)	2-DIMENSIONAL (CROSS-SECTIONAL) VERTICAL · HORIZONTAL	2-DIMENSIONAL · HORIZONTAL	2-DIMENSIONAL VERTICAL	2-DIMENSIONAL	DISPERSION	ADVECTION	MATRIX DIFFUSION	RETARDATION	NON-LIN. ADSORPTION/ DESORPTION	ION-EXCHANGE	(BIO-)TRANSFORMATION/ DEGRADATION	FIRST ORDER RADIOACTIVE DECAY	REACTIONS/HYDROLYSIS (BIO-)CHEMICAL	CHEMICAL COMPLEXATION	VOLATILIZATION	HEAT/ENERGY TRANSPORT	
AT123D	⊖		⊖	⊖	⊖	⊖	⊖		⊖					⊖			⊖		Yeh 1981
LPMM			⊖			⊖	⊖		⊖					⊖					Kent et al. 1989
ONE-D	●	●				⊖	⊖		⊖					⊖					van Genuchten and Alves 1982
Plume (3D)	⊖		⊖		⊖	⊖	⊖		⊖					⊖					Codell et al. 1982
Rocoq			⊖			⊖			⊖										Javendel et al. 1984
SLM	⊖	●	⊖		⊖	⊖	⊖		⊖					⊖					Huyakorn et al. 1987
VHS	●		●		●	●	●												Demonico and Palciauskas 1982
RW-Analyt.			●			●	●		●					●					van der Heijde and Srinivasan 1986
Beaver Soft	●	●	●	●		●	●		●					●					Bear and Verruijt 1987
Kinzelbach	●	●	●	●		●	●		●	●		●		●					Kinzelbach 1986
Walton 35	●		●			●	●		●					●					Walton 1985
Solute	●		●		●	●	●		●					●					Goltin 1985
Femtran				●		●								●					Martinez 1985
Femwater/Femwaste				●		●	●		●					●					Yeh 1987, Yeh, and Ward 1981
Perlie			●	●		●	●		●					●				●	Runchal et al. 1985
GS2/GS3			●	●	●	●	●		●					●					Davis and Segol 1986
PRZM		●				●	●		●	●	●	●					●		Carsel et al. 1984
SESOIL		●				●			●	●		●			●		●		Bonazountas and Wagner 1984
SUMATRA-1		●				●	●		●	●	●	●	●						van Genuchten 1978
SUTRA			●	●		●	●		●	●				●				●	Voss 1984
TRIPM				●		●	●		●					●					Gureghian 1985
CFEST			●	●	●	●	●		●					●				●	Gupta et al. 1987
FEWA/FEMA			●			●	●		●					●					Yeh and Huff 1986
HST3D					●	●	●		●	●				●				●	Kipp 1987
MOC(USGS 2-D)			●	●		●	●		●	●				●					Konikow and Bredehoeft 1978
MOC DENSE			●	●		●	●												Sanford and Konikow 1985
MOC NRC			●	●		●	●		●	●				●					Tracy 1982
RWSTM			●			●	●		●					●					Prickett et al. 1981
SWENT			●	●	●	●	●		●					●				●	Intera 1983
SWFT II			●	●	●	●	●	●	●	●	●	●		●	●			●	Reeves et al. 1986
TRACR 3D					●	●	●	●	●					●					Travis 1984
TRAFRAP/WT	●	●	●	●		●	●	●	●					●				●	Huyakorn et al. 1987
BIOPLUME-II			●			●	●		●	●		●		●					Rifai et al. 1987
PESTAN		●				●	●		●	●				●					Enfield et al. 1982
HELP		●				●				●									See table 3-14

*NON-AQUEOUS PHASE LIQUIDS 1) FOR UNSATURATED ZONE ONLY.

Table 3-15. (Continued)

Model	BOUNDARY/SOURCE CHARACTERISTICS: POINT SOURCE	LINE SOURCE	SPECIFIED CONCENTRATIONS	LIMITED AREA OR VOLUME SOURCE	AREALLY DISTRIBUTED SOURCE	CAPABILITIES: SPECIFIED SOURCE RATE	CONTAMINANT MIGRATE OF RELEASE TO GROUNDWATER FROM UNSATURATED ZONE	CONTAMINANT PLUME EFFECT	AS A FUNCTION OF DEPTH FROM SURFACE	CONTAMINANT CONCENTRATIONS AS A FUNCTION OF DISTANCE FROM SOURCE	CONTINUOUSLY DISTRIBUTED IN SPACE	SELECTED POINTS OR CELLS	AS AVERAGE AT	PROFILES AT	REFERENCE CITATION
AT123D	●	●	●		●	●		●	●	●	●			●	Yeh 1981
LPMM	●				●			●	●		●			●	Kent et al. 1985
ONE-D	●				●	●			●		●			●	van Genuchten and Alves 1982
Plume (3D)	●	●			●			●	●	●	●			●	Cedell et al. 1982
Reseq	●	●	●		●	●		●	●		●			●	Javendel et al. 1984
SLM	●	●	●		●	●	●	●	●	●	●			●	HuyakorN et al. 1987
VHS	●					●		●	●	●	●			●	Domenico and Palciauskas 1982
RW-Analyt.	●	●	●		●	●		●	●				●	●	van der Heijde and Srinivasan 1986
Beaver Soft	●	●	●		●	●		●	●			●	●	●	Beer and Verruijt 1987
Kinzelbach	●	●	●	●	●	●		●	●				●	●	Kinzelbach 1986
Walton 3S	●				●	●		●	●			●			Walton 1985
Solute	●				●	●		●	●	●		●		●	Seijin 1985
Femtran	●	●			●	●	●			●			●	●	Martinez 1985
Femwater/Femwaste	●	●			●	●	●		●	●			●	●	Yeh 1987, Yeh, and Ward 1981
Perflo	●	●	●	●	●	●		●	●	●			●	●	Rumchal et al. 1985
GS2/GS3	●	●	●	●	●	●	●	●	●	●			●	●	Davis and Segol 1985
PRZM	●				●	●	●			●			●	●	Carsel et al. 1984
SESOIL	●				●	●	●			●					Bonazountas and Wagner 1984
SUMATRA-1	●				●	●	●			●			●	●	van Genuchten 1978
SUTRA	●	●	●	●	●	●	●	●	●	●			●	●	Voss 1984
TRIPM	●	●			●	●	●		●	●			●	●	Gureghian 1983
CFEST	●	●	●	●	●	●		●	●	●			●	●	Gupta et al. 1987
FEWA/FEMA	●	●	●	●	●	●		●	●				●	●	Yeh and Huff 1985
HST3D	●	●	●	●	●	●		●	●	●			●	●	Kipp 1987
MOC(USGS 2-D)	●	●	●		●	●		●	●	●			●	●	Konikow and Bredehoeft 1978
MOC DENSE	●	●	●		●	●		●	●				●	●	Sanford and Konikow 1985
MOC NRC	●	●	●		●	●		●	●	●			●	●	Tracy 1982
RWSTM	●	●	●		●	●		●	●				●	●	Prickett et al. 1981
SWENT	●	●	●	●	●	●		●	●	●			●	●	Intera 1983
SWIFT II	●	●	●	●	●	●		●	●	●			●	●	Reeves et al. 1986
TRACR 3D	●	●	●	●	●	●	●	●	●	●			●	●	Travis 1984
TRAFRAP/WT	●	●	●	●	●	●		●	●	●			●	●	Huyakorn et al. 1987
BIOPLUME-II	●	●	●		●	●		●	●	●			●	●	Rifai et al. 1987
PESTAN	●						●								Enfield et al. 1982
HELP	●						●								See table 3-14

*NON-AQUEOUS PHASE LIQUIDS 1) FOR UNSATURATED ZONE ONLY.

Table 3-16. Data Requirements for Unsaturated Zone and Ground-Water Fate Models

	SOIL TYPES	SOIL PERMEABILITY/HYDRAULIC CONDUCTIVITIES	ORGANIC CARBON CONTENT	SOIL BULK DENSITY	CLAY CONTENT	ION EXCHANGE CAPACITY	AQUIFER THICKNESS/DIMENSIONS/RATIO TO TOTAL DEPTH	AQUIFER ELEVATIONS/HEAD PATTERNS/HYDRAULIC GRADIENT	BROADBASTER FLOW RATES	EVAPOTRANSPIRATION RATES	PRECIPITATION RATES	TEMPERATURE CURVES	SOIL MOISTURE	VEGETATIVE COVER	ADSORPTION RATES	ADSORPTION COEFFICIENTS	NATURAL RECHARGE RATES (I.E. DUE TO RAINFALL) ARTIFICIAL RECHARGE RATES (I.E. DUE TO AQUIFER USE, PUMPING)	SITE AREA, TERRAIN, SLOPE PARAMETERS	EXPOSURE POINT COORDINATES OR GRID	RUNOFF RATES	RELEASE MECHANISM/PARAMETERS	VARIABLE RELEASE RATES	SUBSTANCE PHYSICAL/CHEMICAL PROPERTIES	TIME STEP INCREMENT	SUBSTANCE DECAY CONSTANTS	PRESENCE OF CONSTITUENTS	PARTITION COEFFICIENTS	RETARDATION COEFFICIENTS	BACKGROUND OR INITIAL CONCENTRATIONS
SESOIL	●	●	●	●	●	●	●	●			●	●	●	●	●	●			●	●	●		●	●		●	●	●	●	●	●
PESTAN		●	●		●			●			●	●			●	●	●		●		●			●		●	●		●	●	
PRZM	●	●	●	●	●	●	●	●			●	●	●		●		●		●	●	●			●	●	●	●		●	●	●
HELP			◐	◐	◐						◐	◐							●	◐	◐		◐	◐		●					
RWSTM-PLASM		●	●		●			●	◐	◐		●					●	●	●			●		●	●					◐	◐
CFEST & UNSAT-1D	◐	●	●		●			●	◐		●	●	●		●	●	●	●	●		●			●			●	●		●	●
SWIFT		●	●						●	●			●				●	●	●				●	●	●	●				●	●
[illegible]		◐	◐					◐	◐	◐							◐		◐				◐				◐			◐	
FEMWASTE & FEMWATER		●	●		●				●	●		●					●		●						●		●			●	
MOC		●	●					●	●								●	●				●			●						●
AT1230		●	●		●			●	●								●	●				●	●	●	●	●	●			●	●

SOURCES: USEPA 1982b; Brown et al. 1983; Kuis et al. 1983; Versar 1983.

one of three different ways with respect to ground-water flow; area sources, also aligned in one of three different configurations; or a volume source (existing plume). Release types can be instantaneous, longer-term but finite, or constant. Aquitard locations can be specified below or on both sides of the aquifer in any configuration; or the aquifer can be treated as infinite in all directions. Advection and dispersion transports are simulated. Losses resulting from volatilization, degradation, and adsorption are modeled. The model predicts contaminant movement in one, two, or three dimensions (Yeh 1981).

Use of AT123D requires the following information: dispersion coefficients in horizontal, vertical, and longitudinal direction; geometry of the aquifer, especially regarding configuration of aquitards; soil properties, including bulk density, effective porosity, hydraulic conductivity (permeability); source type; and release duration and strength, soil-waste stream partition coefficient, hydraulic gradients, and an overall decay constant (or soil half-life figures) for the substance studied (Yeh 1981).

The model determines contaminant concentration at any point, at a downstream and lateral distance and depth specified by the user, as a function of time from the beginning of source release.

AT123D can be accessed through the GEMS system (see Section 3.1). It is written in FORTRAN and can be installed on a wide range of computer types.

In addition, the Office of Solid Waste (OSW) has developed a national model that uses the Monte Carlo simulation for relisting hazardous wastes on a generic basis. This FORTRAN computer model is a three-dimensional advective-dispersive transport model. The model currently considers the mechanisms of hydrolysis, dispersion, and rainfall recharge into the ground-water plume. OSW is using the model to back-calculate from a health-based standard at the exposed population well to an acceptable on-site leachate concentration. If a treated waste produces leachate with a contaminant concentration below the acceptable concentration, then it is considered protective of the public health.

The model currently uses the HELP model to provide leachate release rates. Leachate strength (concentration) is provided by the Toxicity Characteristic Leaching Procedure (TCLP). OSW plans to add the geochemical model MINTEQ to handle metal speciation. Biodegradation processes are being evaluated for incorporation into the model.

Since EPA's model is a national model that uses a generic environment, the data requirements are minimal. The model approximates an average environment by making multiple runs (typically several thousand runs for each chemical constituent) with varying environmental data. By applying this approach, called a Monte Carlo simulation, one can model the dilution potential of all possible sites as a cumulative frequency distribution versus expected concentration at an exposed population well. The extent to which a particular CERCLA site matches the OSW model depends on the closeness of site characteristics and the model assumptions. If a particular CERCLA site has adequate hydrogeologic data and satisfies the model assumptions, the model can be used for site-specific analyses. Before final assessment of the desired level of cleanup, however, application of the model on a site-specific basis will typically be required. Generic modeling is appropriate for OSW's purposes, but may suggest cleanup levels beyond those necessary at a particular site. Preliminary work or screening-level efforts at CERCLA sites where adequate, good quality hydrogeologic data do not exist can benefit from the model's minimal data requirements for site-specific environmental parameters.

The model is being updated to incorporate flow through fractured media and the unsaturated zone. The data base for MINTEQ is being enlarged to handle additional metals, and more data are being collected to validate the model results.

Since OSW's model uses a Monte Carlo simulated environment, it should be applied with this limitation in mind. Other limitations in the use of this model derive from two sources: (1) limitations in the scope of the model, and (2) specific modeling choices made so that the model would support OSW's requirements. The model's scope is limited by the leachate release algorithm HELP, which models soluble toxic constituents dissolving into percolating rainwater and moving with that water. It does not address percolation of organic fluids into the ground or associated leaching by concentrated organics.

Additionally, the TCLP does not fully predict leachate concentrations due to leaching with water containing dissolved solvents. It does assume the presence of acetic acid in leach water, thereby providing some measure of hydrophobic solubility. Although HELP can model a variety of landfill cover situations, OSW's requirements were such that it modeled a landfill with a failed liner but an intact (aged) cover. The permeability of the hypothetical cover was chosen at 1×10^{-6} cm/sec to represent an aged (deteriorated) cover with an initial permeability of 1×10^{-7} cm/sec. OSW states that it found the range of permeabilities for aged clay actually to be between 1.4×10^{-6} and 43×10^{-6} (USEPA 1986). For CERCLA sites, selection of a permeability within that range may be more appropriate. Also, many CERCLA sites do not have a cover, or the cover may be breached. In either case, the mass flux leaving the site will be considerably larger. Even if the site has an intact cover, one may wish to predict long-term potential

releases and also to consider the eventual subsidence and breaching that may occur in the future.

Pesticide Root Zone Model (PRZM) (Carsel et al., 1984) simulates the vertical movement of pesticides in unsaturated soil, both within and below the plant root zone, and extending to the water table using generally available input data that are reasonable in spatial and temporal requirements. The model consists of hydrology and chemical transport components that simulate runoff, erosion, plant uptake, leaching, decay, foliar wash off, and volatilization (implicitly) of a pesticide. Predictions can be made daily, monthly, or annually.

3.5.4 Short- and Long-Term Concentration Calculations

Long-term average ground-water concentrations of contaminants at exposure points are a function of the concentration profile over the time period of study, which are, in turn, a function of hydrologic fluctuations, release rate fluctuations, and the effectiveness of remedial actions. Average concentration values are obtained from steady-state methods. Several of the in-depth analysis models tabulated in Section 3.5.3 accept time-weighted input data, and provide long-term average concentrations, as well as the concentration profile as a function of time.

Short-term concentrations at exposure points are obtained by examining the ground-water concentration profile at the selected exposure point over time, and identifiying of the period of maximum concentration.

3.6 Biotic Pathways

3.6.1 Estimation Procedures

After the fate of a contaminant in air, water, and ground water has been estimated, one can assess its fate in biotic populations. Using the ambient concentration data developed for each of these media, a determination is made whether any biotic populations that can potentially serve as pathways for human exposure to hazardous materials (i.e., vector organisms) are within zones of elevated hazardous material concentrations. Such vector populations may include agricultural crops; agricultural livestock; fish, shellfish, or crustaceans that are important commercial or sport species; and game populations in hunting areas.

In assessing the biological fate of hazardous materials, the following processes, which determine the rate of introduction of hazardous material to and the final concentration of hazardous material within vector organisms, should be considered:

- The concentration of hazardous material in environmental media containing or supporting vector organisms.
- The metabolic rate of the vector organisms. Metabolic rates are functions of several environmental parameters including temperature and the availability of sunlight, oxygen, nutrients, and water or other factors.
- Substance bioavailability; the affinity of each hazardous substance for partitioning into the organic phase or its availability for other forms of uptake. The bioavailability of each substance differs, as does that of various chemical species of an individual substance; the octanol/water partition coefficient is an indication of this parameter. Bioavailability of a given substance can vary with environmental conditions. Factors that influence the physiochemical speciation of substances, and thus their bioavailability, include salinity, pH, Eh, organic carbon concentration, and temperature.
- Characteristics of species metabolic processes. These characteristics differ among species and include feeding habits and ability to metabolically degrade, store, and eliminate the substance. Bioconcentration factors (or BCFs, the ratios of organism tissue concentration to ambient environmental concentration) for many species and hazardous substances have been empirically determined and are discussed below.

Consider the following transport mechanisms in assessing the distribution of hazardous substances within the biologic medium and identifying the potential points of human exposure:

- Transport and distribution of vector organisms as a result of human commercial or sport activity.
- Migration of organisms, or movement of these organisms with advective flow of environmental substrate media.
- Movement of contaminants through the food chain. This mechanism often results in very high concentrations of hazardous materials in the tissue of higher trophic level organisms within and without contaminated areas.

General theoretical relationships between the above factors and concentrations of hazardous substances at human exposure points are not available. This is because such relationships are highly specific to individual ecologies, biotic species, hazardous substances, and human activities associated with involved biotic species.

For this reason, the assessment of biotic concentrations of hazardous substances at human exposure points is limited to the qualitative identification of major pathways, and the rough quantification of exposure levels wherever some means of relating ambient soil, water, or air concentrations to edible tissue concentrations are available.

The available methods of estimating tissue concentrations in aquatic animals, terrestrial animals, and terrestrial plants are discussed in the following sections.

3.6.1.1 Aquatic Animals

Because aquatic animals are immersed in the contaminated water medium to which they are exposed, it is commonly assumed that tissue contaminant concentrations are a function of contaminant equilibrium partitioning between water and organic tissue, and are therefore directly related to contaminant ambient water concentrations. The bioconcentration factor (BCF) represents the ratio of aquatic animal tissue concentration to water concentration. This ratio is highly contaminant-specific and is also dependent on the aquatic species and on site parameters.

The most reliable source of aquatic animal BCF values is monitoring data for the site. Wherever water concentrations and biotic tissue concentrations have been surveyed simultaneously, a site-specific BCF can be calculated for the species and substance involved (assuming water column concentration values represent relatively steady concentrations over at least the previous several weeks, and not short-term high or low concentrations). This BCF can be used to project changes in tissue concentrations resulting from projected changes in ambient water concentrations of the involved hazardous substance.

In cases where site monitoring data are insufficient for development of a BCF, one can use the BCF values reported in technical literature. A substantial amount of research is available regarding the bioconcentration of hazardous substances, especially in aquatic organisms (see USEPA Office of Water Regulations and Standards: Ambient Water Quality Criteria documents, for a review of research current to 1980; or Verschueren 1984; Dawson, English, and Petty 1980; Mabey at al. 1982; and Callahan et al. 1979 for BCF factors). Exercise care to match contaminants, species, and site conditions (e.g., temperature, pH, water salinity) for which reported BCF values were measured with conditions at the site. BCF values for different species or contaminants or those measured under dissimilar conditions may not be applicable.

A third alternative for derivation of BCF values is to calculate these values based on the structure or physiochemical properties of the hazardous substance. See Lyman et al. (1982), Kenaga and Goring (1978), and Veith et al. (1980) for instructions on BCF estimation procedures.

3.6.1.2 Terrestrial Animals

Little data are available allowing the quantification of contaminant concentrations in edible terrestrial animal tissue based on ambient environmental concentrations. Kenaga (1980) compiled and studied data comparing dietary concentrations of several organic compounds with the concentration of these compounds in the fat of beef cattle. He found that the fat/diet BCFs for these compounds correlate reasonably well with the water solubility (negative correlation) and octanol-water partition coefficient (positive correlation) of these compounds. BCFs could only be predicted within three to four orders of magnitude, however. This method of tissue concentration estimation must be considered semiquantitative at best.

Human exposure to contaminants through the terrestrial animal pathway can be reliably determined only through identification of potential vector organisms and exposure points, and through a sampling and analysis program for determining tissue concentrations at these exposure points.

3.6.1.3 Terrestrial Plants

Plant adsorption of environmental contaminants has been studied by various researchers, and some data are available regarding the uptake of pesticides and other contaminants by edible crops. These data cover specific crop uptake of specific contaminants (see CDHS 1985 for a review of pesticide research), however, and no relationships allowing reliable extrapolation of soil/plant tissue concentration ratios are presently identified. Where plant/soil BCF data are available in the technical literature for the specific plant species, contaminant, soil type, and tissue type of concern in a Superfund exposure assessment, these BCF data can be used for a semiquantitative estimation of edible tissue concentrations.

As is the case with terrestrial animals, the most reliable technique for assessing contaminant concentrations at points of human exposure to plant tissue is the identification of potential vector organisms and exposure points, and the surveying of tissue contaminant concentration in these organisms.

Chapter 4
Uncertainty in the Analysis

This chapter provides a brief introduction to the evaluation of uncertainties inherent in the exposure assessment process. When applying the exposure assessment tools outlined in the preceding sections, uncertainty may be a factor at each step. Such uncertainty can involve variations in the values of variables used as input to a given model, the accuracy with which the model itself represents actual environmental processes, and the manner in which the exposure scenario is developed. Each of these categories of potential uncertainty is discussed below. Once the exposure assessment is completed, its results must be reviewed and evaluated to identify the degree of uncertainty involved. This factor should then be considered when using the assessment results for remedial decisionmaking.

The following discussions focus on the uncertainties of assessing the average daily exposures to toxic chemicals; uncertainties related to the human health response to these exposures are not discussed. The information provided here does not constitute a comprehensive treatment of uncertainties in the exposure assessment process. It is intended to make the analyst aware of the categories of uncertainties that may be involved in exposure assessments. In-depth guidance for the execution of uncertainty analyses is provided in various references in the literature. Specifically, the analyst may wish to review the following sources of information concerning various aspects of uncertainty analysis pertinent to the exposure assessment process:

- Cohen (1950)
- Eisenhart (1968)
- Henrion and Morgan (1984)
- Hoffman et al. (1984)
- Kleijnen (1974)
- Morgan et al. (1984)
- Rubinstein (1981)
- USEPA (1987e)

4.1 Sources of Uncertainty

4.1.1 Input Variable Uncertainty

Most of the analytical procedures presented in this manual are quantitative in nature, and their results may be highly dependent upon the accuracy of the input variables used. For example, hydraulic conductivity and other parameters that determine the velocity of ground water and the contaminants that it may carry can vary significantly over relatively short distances, thereby affecting one's ability to estimate average contaminant velocities with confidence. Similarly, the presence of hydrogeologic heterogeneities can affect the speed with which contaminants arrive at a given well from their point of release and also their direction of travel. Often, the presence of such heterogeneities may be unknown. Thus, the accuracy with which values for such parameters can be quantified is critical to the degree of confidence that the decisionmaker has in the assessment results.

Most scientific computation involves a limited number of input variables, which are tied together by a model to provide the desired output. The input parameters can be broadly classified into the following categories: constants, state variables, and natural variables.

A constant has a single value irrespective of the nature of other variables. In some cases, the variability of a parameter may be so small that it can be considered constant. In other cases, even if the value varies, its effect on the final answer may be minimal. The results are not sensitive to variation in that parameter's value.

A state variable is one that has a fixed value, but that value is not known accurately. The errors in such variables are due to limitations in experimental techniques. A relevant example is the octanol:water partition coefficient. While this has a single value for a given system, some degree of uncertainty is introduced through experimental errors. In some instances the values of state variables are estimated rather than measured; therefore, the uncertainties for such values are even higher.

A natural variable is one that can exhibit different values. An example is soil porosity, which can exhibit different values within a range because the soil matrix varies with location, and because a given area may include many soil types.

If the actual values for such variables are not accurately known for the location in question, the estimated exposure may be significantly in error. This problem is illustrated by a study where the values of parameters needed to calculate the velocity of a solute in ground water were varied randomly, using Monte Carlo simulation techniques (Mercer, Silka, and Faust 1985). This analysis determined that the velocity estimates may vary over four orders of magnitude.

The selection of accurate input parameters is essential to estimate the contaminant velocity and other components of the exposure assessment. Often, however, the analyst will not be able to determine the value of such parameters with absolute certainty. It is important that one be aware of the type and degree of uncertainties involved at each stage of the analysis, and interpret the results obtained accordingly.

The different values of input parameters that are measured many times can be expressed as a parameter distribution. A parameter distribution typically appears as a bell-shaped curve. The mode, or the most likely value, is represented by the peak of the bell-shaped curve. The tails to either side represent the relative frequency of times when the measured values are greater or less than the mode. For a parameter that varies considerably, the bell-shaped curve will be wide (standard deviation is large). For those that do not vary appreciably, it will be narrow (standard deviation is small).

Input parameter distributions can be used to generate the output parameter distribution. The shape of the parameter distribution conveys the degree of uncertainty of the parameter (input or output). This is the most rigorous way to define the uncertainty of the predicted output parameter; however, it is used infrequently in the environmental field due to the lack of input parameter distributions upon which to base the predicted output parameter distribution. This subject will be discussed further in the section on the Monte Carlo technique.

In the environmental field, the methods used for discussing the degree of uncertainty are often qualitative rather than quantitative. Qualitative methods involve discussing whether the data are thought to be representative or not. Some exposure modeling is done based on literature values rather than measured values. In such cases the degree of certainty may be expressed as whether the estimate was based on literature values or measured values, not on how well defined the distribution of the parameter is. Some exposure estimates are based on estimated parameters; the qualitative statement that the exposure was based on estimated parameters defines the certainty in a qualitative manner.

4.2 Modeling Uncertainty

4.2.1 Model Simplification

The degree to which a specific contaminant transport and fate model accurately represents the actual conditions that are present in the environment constitutes a large source of potential uncertainty. The analyst must choose the model that addresses the appropriate aspects of interest.

Models are typically simplifications of the complexities of reality. There is some accuracy lost when making these simplifications. While such loss may be small in some cases, in others it may be unacceptably large. Two assumptions that illustrate this idea are the assumptions of homogeneous soils and isotropic soils for ground-water models. In most cases, these assumptions do not materially change the answer. If the soil under the site has layer cake stratigraphy, the assumption of homogeneity is invalid. Typically, most cases will be in-between the two extremes of homogeneous soils and completely non-homogeneous soils. The analyst will have to decide if the assumptions are valid for each case.

In some cases the simplification of the real world into an actual model is acceptable and, although producing uncertainty, it is a necessary evil. There is a point at which the level of the discrepancy between the model and the real world constitutes an error in the use of the model and not an acceptable simplification that is necessary to model a complicated real world. At this point, the deviation is an error and not an uncertain prediction.

4.2.2 Averaging Hydraulic Conductivities

An example of this would be the modeling of ground water flow by averaging the hydraulic conductivities across all aquifer materials. For contaminant transport modeling, this would constitute an error; however, for modeling well production, this is an accepted practice. Ground water modeling with numbers has been occurring for the last 100 years. For the first 90 years of this period, most of the modeling was for water supply; contaminant migration was not modeled. The practice of averaging the hydraulic conductivities across the cross-sectional area of the aquifer produced answers that had high certainties when predicting the volume of water that could be produced by a well during a period of time. Some modelers applied this technique to the problem of modeling contaminant migration and produced erroneous results. Although they were accustomed to this practice, it was not acceptable in this case.

Modeling contaminant migration requires that areas of different hydraulic conductivity be treated separately (sometimes it is not possible to differentiate the areas and the model results must be viewed as less certain). For example, if the site overlies a sand layer and a clay layer, the analyst should model the two

layers separately. The result of the separate modeling will show that the time of arrival in the sand is much sooner than in the clay layer. Effectively the majority of the contaminant mass would migrate through the sand layer and hardly any would use the clay layer for migration. Assuming an average hydraulic conductivity would predict a time delay between release and arrival that is 100 to 1000 times too long. Such uncertainties, however, constitute an error of approach, and are not unresolvable uncertainties.

4.2.3 Dispersion Simulation

Different ground-water models simulate dispersion in different ways. The degree to which a particular model accurately models the dispersion at a given site affects the accuracy of using that model for that site. Ground water dispersion modeling is a young field and the state of the art is rapidly advancing. The analyst should become familiar with the dispersion simulation technique for each model he/she uses.

Also, some ground water models presume an aquifer of infinite depth, while some model a finite aquifer depth. Contaminants dispersing in an aquifer of finite depth will effectively reflect off the lower aquitard and cause the resulting downstream concentrations to be larger. Use of a model appropriate to the constraints of the site is necessary for accurate modeling of the drop-off in contaminant concentration with travel distance. Additionally, some models will simulate lateral constraints of the aquifer to model this limitation on the reduction in downstream concentrations.

Dispersion modeling in air and surface water has been performed for a much longer time, and as such, the methods for modeling dispersion have coalesced into a consistent approach. However, limitations on the extent of dispersion for air modeling can vary. For example, a valley model will simulate the constraint of lateral dispersion by the valley walls. A model that handles inversions will simulate the build-up of contaminant concentration due to limited vertical mixing. Surface water models may vary on the approach they take to modeling initial mixing. Some surface water models use compartments to manage the modeling task. If the modeler uses a small number of large compartments, small scale effects may not be accurately modeled and the results will be less certain.

4.2.4 Numerical Models and Analytical Models

Different types of models provide varying accuracy in different situations. Two types of models are numerical (finite-element) and analytical models. Neither is best in all cases, but one is usually better in a given situation. The numerical models are typically more difficult to use, and thus ease of use may enter into the decision of model selection.

Analytical models often involve mathematical simplifications. These simplifications are made in order to find a closed-form solution. In most cases the accuracy lost is negligible; however, in extreme cases the inaccuracy will be large.

Typically, analytical models require less computer time than do numerical models. If the grid is large, a numerical model requires a substantial amount of computer time for each run. Numerical models typically require more input data. Different program needs cause different questions to be raised. A preliminary scoping problem will rarely require a numerical model; conversely, a problem that requires maximum defensibility will suggest that the additional data and operational burdens of a numerical model are justified in light of the greater certainty of the output.

In cases where the question involves simulating what will happen in typical generic situations across the country, an analytical model will give a better picture than a numerical model. Numerical models address site-specific conditions better than do analytical models; they do not necessarily model a typical situation with any increased accuracy.

4.2.5 Chemical Degradation Simulation

Some models do not describe all of the processes that may potentially occur. For example, degradation is not accounted for in some models. If the contaminant is extremely refractory (i.e., does not degrade), this limitation will not materially affect the answer. If the contaminant degrades quickly, however, this limitation will cause the model results to be in substantial error. Some models simulate the effect on the reaction rate kinetics of two concentrations while some use only one concentration. The simpler approach of 1st order reaction kinetics is acceptable if the other concentration does not vary appreciably, and is less accurate if both the concentrations vary substantially. The analyst must rely on his/her judgment to ensure that the uncertainty is minimized.

4.2.6 Model Operational Parameters

Certain modeling parameters specified by the analyst can have a profound effect on the accuracy and viability of the output. An example is the parameter "time step." Time step is used on iterative models. Models may either calculate an answer explicitly or they may determine their solution with a successive iteration approach. For iterative models, the analyst will have to make many model runs, and not stop until he/she has a good run. The challenge of choosing an appropriate time step is that both too large and too small time steps cause inaccuracies. The analyst must find the optimum size for the time step. A time step that is too small causes numerical error

propagation (see below), while one that is too large causes a less accurate calculation of each step.

Numerical error propagation in iterative models can cause inaccurate answers. If the analyst uses too many iterations, the truncation error of digital representation of numbers can build upon the successive iterations and produce output that is totally erroneous. The degree of error that can be present can make the output totally meaningless. For example, the estimated output concentrations can include concentrations that are greater than a million PPM or concentrations that are negative. Clearly, concentrations in these ranges signify a bad run. The analyst must also watch out for iteration errors that produce errors that are less obvious and, hence, there is the possibility that the analyst will not be aware of their occurrence. Conversely, the analyst may choose too few iterations and the resulting time step between each iteration then becomes too large. In this case, the model will inaccurately calculate each step. The analyst must become familiar with the models he/she is using so as to stay in the safe area between the two extremes. Knowing the precise limits is difficult, but staying between them is important.

4.2.7 Source Shape

The degree to which the shape of the source is modeled can effect uncertainty. For example, if the analyst uses a point source model to model an area source, the nearby concentrations will be less accurate than they would be if the analyst used an area source model. Line sources and volume sources can provide the same problem. At large distances from the source, the effect of the shape of the source is less important, and may often be neglected. Some sources are best modeled as a vertical line source and some are best modeled as a horizontal line source; hence, orientation is a factor as well as shape. It is a matter of fit between the model and the actual site rather than choosing the best source shape for all cases.

4.2.8 Steady State Modeling

Use of a steady-state model to model a true steady-state scenario provides accurate results. Use of a steady-state model to model a truly dynamic scenario can produce inaccurate answers. In most cases, the analyst will have to make a judgment as to whether the actual scenario is close enough to steady state to justify using a steady-state model. The analyst must match the model to the question being asked, and to the details of the specific site, in order to minimize the uncertainty of the output.

4.2.9 Number of Dimensions Addressed by the Model

Choice of a one-, two- or three-dimensional model can affect the uncertainty of the results. Neither is best in all cases and, typically, one is preferred in a given site-specific scenario. The three-dimensional model generally has less uncertainty than the one- or two-dimensional models, but, this is not always the case. For example, when modeling the migration of contaminants in ground water through a 10-foot thick aquifer, a two-dimensional model will produce more certain results than the blind application of a three-dimensional model. It is not just a trade-off between difficulty of the model and quality of the output, but a matching situation as well.

4.3 Scenario Uncertainty

The analyst needs to be aware of uncertainties that result from using conservative assumptions when data are lacking. While it is traditional in exposure assessment to make conservative assumptions in the absence of data, such assumptions must be reasonable and the assessment results must be interpreted with caution. Use of reasonably conservative assumptions at each step may produce cumulative assessment results that are overly conservative and thus unreasonable.

In addition, conceptual errors may result in the use of assumptions that affect the selection of the modeling technique applied to the exposure assessment. For example, using a three-dimensional model in situations where the aquifer thickness is not "large" in relation to the areal extent of contamination would not be appropriate. Thus, the concepts upon which the exposure scenario is based must be carefully considered to make sure that they adequately reflect the situation under evaluation.

Quantitative descriptions of scenario uncertainty are often impractical, and qualitative descriptions of the level of uncertainty are more common for the young, and developing, field of exposure assessment. Any exposure prediction has cases of overstatement and understatement of risk. Where possible, the understatements and overstatements of risk are minimized. Where this is not possible, the analyst attempts to balance them so as to produce a prediction that is most realistic.

4.4 Approaches for Dealing with Uncertainty

4.4.1 Sensitivity Appraisals

Variation in the values of input parameters causes variation in the values of the output parameters. The ratio of the input parameter variation to the output parameter variation will be different for parameters in different parts of the equation. Sensitivity appraisals involve assessing which parameters have the highest ratios and which have the lowest. The accuracy of parameters that have the largest effect on the accuracy of the output parameters should be high, while parameters that have only a small effect on the accuracy of the output parameters can be estimated

or determined by less accurate and less costly methods.

Sensitivity appraisals can be quantitative or qualitative. A quantitative sensitivity appraisal involves plotting the output parameter as a function of variation of a single input parameter, while holding all of the other input parameters constant. As one can imagine, there may be a different functional relationship between the output parameter and the varying input parameter for each combination of fixed input parameters. For complex models the approach can become overwhelming. Typically, the analyst will be able to interpret the equation and set up the fixed input variables so as to minimize the number of functional relationships produced. However, it may still be burdensome, and it may produce results that are more precise than necessary.

In the environmental modeling field, the qualitative approach has strong advantages over a quantitative approach. The qualitative approach involves inspecting the model's equations, and ascertaining which input variables are the most sensitive. This is usually done by visual inspection, with an understanding of the mathematical relationships in the equation. For example, if one input parameter multiplies all the other terms, the analyst can expect the input parameter to have a sensitivity ratio of one. If the input parameter is the exponent of the other terms, the analyst can expect this parameter to have a very high sensitivity ratio. If the input parameter is part of a separate term that is added to the rest of the equation, and it is multiplied by a constant of low value, the input parameter can be assumed to have a low sensitivity ratio. A qualitative appraisal is usually the most efficient technique for determining the input parameter accuracy needs.

4.4.2 Monte-Carlo Simulations

The Monte-Carlo technique involves running a model a large number of times with varying input parameters. The values for the input parameters are chosen from the parameter distributions, with its relative frequency of a particular value being used being equal to the relative frequency in the parameter distribution. This is based on the assumption that the input variables vary independently from each other. This technique generates an output parameter distribution, which provides a mode and a statement of the uncertainty associated with the prediction.

One difficulty with this technique is the assumption of independent variation. The input variables are chosen as if there were no relationship among them. If the variables are truly independent, the results are accurate. Typically, however, the variables are related to each other and are, thus, dependent variables. For example, if the two input variables are hydraulic conductivity and hydraulic gradient, the analyst could assume that they are either independent or dependent. The analyst could assume independency because the two variables represent different factors that do not have a direct functional relationship between them. But, if the analyst looked at enough sets of data, the sites with high conductivity would have more gradients that are flat; conversely, the sites with low conductivity would have more gradients that are steep. Thus, the two variables would exhibit covariation and cannot be considered strictly independent. This weakens the validity of using the Monte-Carlo approach.

While it is possible to use input parameter distributions to generate model output distributions using Monte-Carlo simulations, it is usually not possible to get the input parameter distributions. The input parameter distribution shows the variation of parameter values. It must be based on a large number of observations (actual measurements). The environmental field is young and growing. As such, most sampling (to date) falls short of providing the mass of data necessary to generate an input parameter distribution. Faced with this dilemma, some analysts have fallen back on assuming such distribution. Since they do not have a way to gauge the distribution, a uniform distribution from the lowest to highest possible value is assumed. This distribution states that there is an even probability that the value could be any value between the lowest and the highest value of the range.

Assuming an input parameter distribution does not help to reduce uncertainty, however, as the certainty of the output is then a function of the assumed certainty of the input parameter. For example, if you assume that the input parameters are very precise, then the certainty of the output is high. Conversely, if you assume the parameters may have an equal probability to be any value across the range of possible values, the certainty of the output will be low. Using a Monte-Carlo approach with assumed input parameter distributions that are uniform only indicates how accurate the model is at predicting the output parameter when you have no idea what the input parameters are, since models predict output based on the relationship to the input parameters. Thus, using the Monte-Carlo technique to assess the certainty of a model's predictions cannot be done with assumed input parameter distributions.

4.4.3 Using Monitoring Data to Calibrate the Model

One of the best ways to reduce the uncertainty of the predicted parameter is to use monitoring data to calibrate the model. If you have measured contaminant concentrations that are comparable to modeled contaminant concentrations, the analyst can correct for over- or under- predictions. If for example, the measured values are always 90% of the predicted values, the analyst can multiply all of the output values by 90%.

The difficulty of this technique is that the values must be comparable. In many cases the model is being used to predict future events. Current contaminant concentrations can be determined more accurately by monitoring, thus the need for modeling is reduced.

In air and surface water modeling the difference between current and future events is much smaller than for ground water modeling. Air and surface water move more quickly than does ground water. Hence, calibration is a more useful technique in air and surface water modeling than in ground water modeling.

If the ground water model predicts a certain contaminant concentration 1 mile from the source after 20 years, and monitoring shows no contamination at 1 mile from the source, this cannot be used to calibrate the model. The plume may not have reached the point 1 mile away, as of yet. In 20 years, monitoring may very well show the same contaminant concentration that was predicted by the model. Care should be taken to ensure that the monitoring data used to calibrate the model are comparable in time and space.

4.5 Level of Uncertainty Appropriate for Exposure Modeling

There is no one level of certainty that is appropriate for all situations. Each program has different needs, and various parts of a program have diverse needs. A screening level study has less need for accuracy than a court case that will require a substantial sum of money from a PRP. The level of defensibility required will vary from one situation to another

EPA program offices have developed a multi-tiered approach. A desk top model may be sufficient for a first-tier analysis, an analytical model may be sufficient for a second-tier analysis, and a numerical model may be required for a third-tier analysis. For example, the method of screening sites for inclusion on the National Priorities List should be less rigorous than the method of supporting a decision on various site clean-up options. Data requirements will also vary.

Although it would be nice to have maximum accuracy in all cases, it would also imply maximum difficulty in all cases. Clearly, a balance must be found between difficulty and accuracy of the prediction.

4.6 Risk Communication

Once the analyst has completed the modeling task, the results of the task must be communicated to the analyst's supervisor. This information should include the predictions of exposure over time, and it should include some communication regarding the level of uncertainty associated with the prediction. The level of uncertainty can be expressed in a quantitative or qualitative form. Further guidance on risk communication can be found in USEPA (1987e).

A quantitative appraisal of the uncertainty is the most preferable way to express the uncertainty. A quantitative presentation may be an output parameter distribution which tells the most probable value (mode) and the relative probability that the value is larger or smaller than the mode. Or, the presentation may consist of the predicted value and a standard deviation. The standard deviation provides the level of precision or uncertainty. Another approach involves providing the predicted value and the 95% confidence limits. The 95% confidence limits express that 95% of the possible values of the parameter will be between the upper and lower confidence limits. The main catch to precise numerical expression of the uncertainty is the lack of sufficient data upon which to base the quantitative expression of the uncertainty. In the future, it may be possible to use this precise approach.

A qualitative appraisal of the uncertainty is the most viable way to express the level of uncertainty. A qualitative presentation will describe the significant factors that determine the level of uncertainty. The quality of the prediction is a function of the quality of the inputs to the prediction. Major inputs that affect quality are: data precision, model sophistication, and defensibility of the scenario.

Expressing the quality of the data would entail describing the sources of the data. For example: Did the data come from literature values or were the data taken from actual site measurements? Were the data measured by the best available techniques or were they sampled by another technique? Were replicate samples taken? Was the sampling protocol sufficient to obtain representative samples? Are the costs of the sampling program appropriate for the use of the results, or could more expensive data gathering techniques be used?

Expressing the quality of the model used would entail a description of the type of model. For example: Is the model a desk-top calculation, an analytical model, or a numerical model? Has the model been in use for some time or is it new? Is the model a standard model used by the agency or is it new to the agency? Have other people used the model? Does the model address all of the important facets of the situation, or does it neglect some potentially important factors? Has the model been used in court cases before? How good is the model relative to other possible models? Is it the best available model at this point in time? Is the model the most defensible model available? Were monitoring data used to calibrate the model predictions? How comparable were the monitoring data to the model predictions?

Expressing the quality of the scenario is more difficult. Reasonableness of the scenario is important. Use of similar scenarios by the agency in the past is useful information. Questions to ask would include: Was the scenario used in court cases, for rulemaking activity that has been published in the Federal Register, and/or did it receive public comment? Was the public comment favorable or did it bring out potential difficulties? Does the scenario neglect certain exposure routes that have been neglected by the agency in the past?

The important aspect to consider is how good the prediction is, not how imperfect the model is. Modeling is a young field that is rapidly growing. Uncertainties are minimized but never eliminated. Modeling produces state-of-the-art estimates, and nothing more.

Chapter 5
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Appendix A

Analysis of Exposed Human Populations and Exposure Calculation and Integration

Table of Contents

Chapter		Page
1	QUANTITATIVE ANALYSIS OF EXPOSED POPULATIONS	114
	1.1 Introduction	114
	1.2 Exposed Populations Screening	114
	1.3 Quantitative Exposed Populations Analysis	116
	1.4 Identification and Enumeration of Exposed Human Populations	118
	1.4.1 Populations Exposed Through Air	118
	1.4.2 Populations Exposed Through Surface Water or Ground Water	119
	1.4.3 Populations Exposed Through Food	119
	1.4.4 Populations Exposed Through Soil	120
	1.5 Population Characterization	120
	1.6 Activity Analysis	120
2	EXPOSURE CALCULATION AND INTEGRATION	121
	2.1 Inhalation Exposure	122
	2.2 Dermal Exposure	123
	2.3 Ingestion Exposure	128
	2.3.1 Food/Soil	128
	2.3.2 Water	128
	2.4 Exposure Integration	129
3	APPENDIX A REFERENCES	131

Chapter 1
Quantitative Analysis of Exposed Populations

1.1 Introduction

The results of contaminant release and fate analyses provide the basis for assessing exposed populations. This assessment compares environmental contamination data with populations data to determine the likelihood of human contact with contaminants of concern. This chapter details methods useful in evaluating the following components of exposed populations analysis:

1. Identification and enumeration of exposed populations;
2. Characterization of exposed populations; and
3. Analysis of activities that bring populations into contact with contaminants.

Each of these components is detailed in the following subsections.

As with other evaluations, exposed populations analysis begins with a screening assessment, which identifies exposure pathways that are incomplete, i.e., those situations where contaminants are released and migrate from a site, but do not contact human populations and are not likely to do so in the future. Such situations require no further analysis. At the same time, exposed populations screening also points out those exposure pathways that are complete and that will require quantitative analysis to estimate the extent of human exposure.

Data needed to quantify potentially exposed populations are readily available. In essence, all quantitative exposed populations evaluations can be considered in-depth analyses. For each population segment identified in this portion of the exposure assessment process, exposures are quantified and integrated as described in Chapter 2 of this Appendix.

1.2 Exposed Populations Screening

Exposed populations screening is primarily qualitative. This evaluation draws on the results of contaminant fate analysis (presented in Chapter 3) to determine the likelihood and extent of human population contact with contaminants.

Exposed populations screening is guided by the decision network provided in Figure A-1. The following numbered paragraphs each refer to particular numbered boxes in the figure.

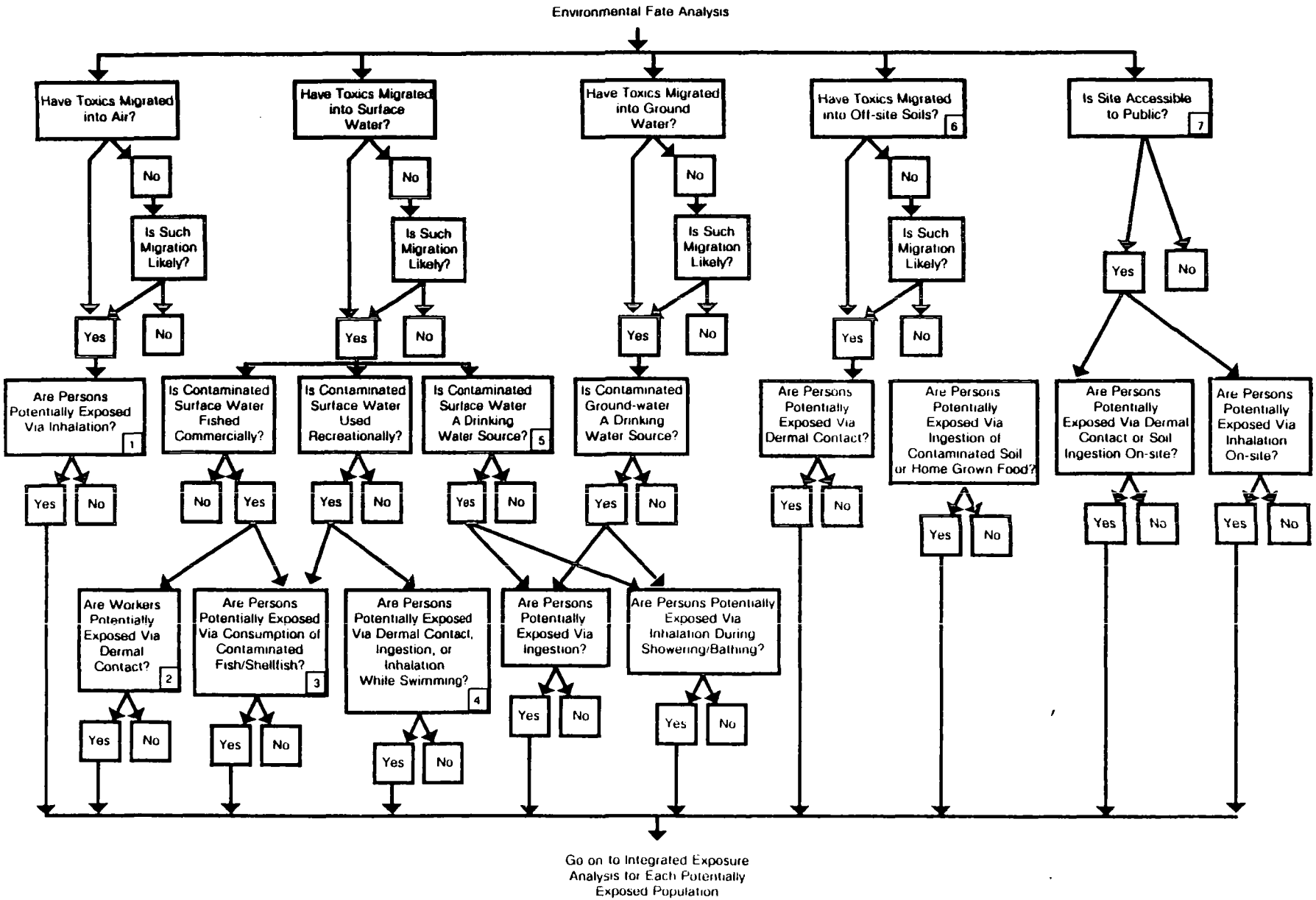
1. Human exposure through inhalation should be evaluated for contaminants that have migrated or may migrate from the site into air. The assessment should consider both contaminated dust and volatile compounds. For screening purposes, comparing contaminant concentration isopleths with maps of the local area will identify the potential for such human population inhalation exposure. The user should realize, however, that exposure can occur in recreational areas as well as in residential, commercial, or industrial areas, and should interpret local area maps accordingly.

2. In cases where surface waterbodies have been contaminated by toxics migrating from a site, the water's potential commercial use as a fish or shellfish source should be evaluated. If the waters are commercially fished, fishermen may be exposed through dermal contact with contaminated water, although such exposure will generally be overshadowed by other exposure mechanisms.

3. In cases where recreationally or commercially caught fish/shellfish are taken from contaminated waters, persons consuming the catch may be exposed. For chemicals that tend to bioaccumulate, consumers may be exposed to contaminant concentrations in fish/shellfish tissue that are many times greater than those present in the water column or sediments. When performing exposed populations screening, the analyst need only determine whether waters identified in the environmental fate analysis as having received contaminants from the hazardous waste site are used commercially or recreationally.

4. Individuals who swim in contaminated waters can experience dermal exposure to toxics over their entire body. In addition, significant quantities of contaminated water may be ingested inadvertently while swimming, and swimmers will be exposed to

Figure A-1. Exposed populations decision network



volatile contaminants in the water through inhalation. Other screening should evaluate the existing or potential degree to which the local population uses contaminated water-bodies (fresh or marine) for swimming.

5. If contaminated ground water or surface water is a source of potable water, the population served may experience considerable ingestion exposure. Similarly, the population may also be exposed to toxics through both dermal absorption and inhalation (of volatiles) while showering or bathing. When undertaking a screening analysis, it is only necessary to determine which residences or commercial/institutional establishments are likely to obtain their potable water from contaminated water sources.

6. If contaminants migrate to off-site soils, persons contacting such soil may be exposed. Individuals who grow their own fruit or vegetables at home may experience additional exposure from ingesting food grown in contaminated soils, as do those consuming contaminated commercially-grown foods. Similarly, livestock that have grazed on contaminated vegetation may constitute a source of ingestion exposure for consumers. Screening analysis should strive to correlate areas of human habitation with areas of contaminated soil, as defined in the environmental fate analysis.

7. Similarly, if direct access to the site is possible, children may be attracted to the location and may directly contact hazardous materials or contaminated soil. Such activity may result in inhalation or dermal exposure, as well as intentional or inadvertent ingestion of contaminated soil. For screening purposes, the proximity of residential areas to the site should indicate the potential for direct access by children.

1.3 Quantitative Exposed Populations Analysis

Quantitative analyses of potentially exposed human populations comprises three distinct steps, which are illustrated in Figure A-2. First, the results of environmental fate analysis are compared with data identifying and enumerating nearby human populations to provide boundaries and quantify the population(s) potentially or actually coming into contact with contaminated air, water, and soil. Populations consuming contaminated food (home grown vegetables, fish) can similarly be identified once the areal extent of contamination is known.

Population characterization, the second step, involves identifying those groups within the exposed population that, because of the specific health effects of some pollutants or factors related to the population itself, would experience a higher risk than would the average population as a result of a given level of exposure. Indeed, the health effects of the contaminants under evaluation will often dictate the need for population characterization. For example, if mutagenic or teratogenic substances are involved, women of childbearing age should be considered a high-risk group. In addition, factors relating to the exposed population may cause certain groups to constitute high-risk subpopulations. These include:

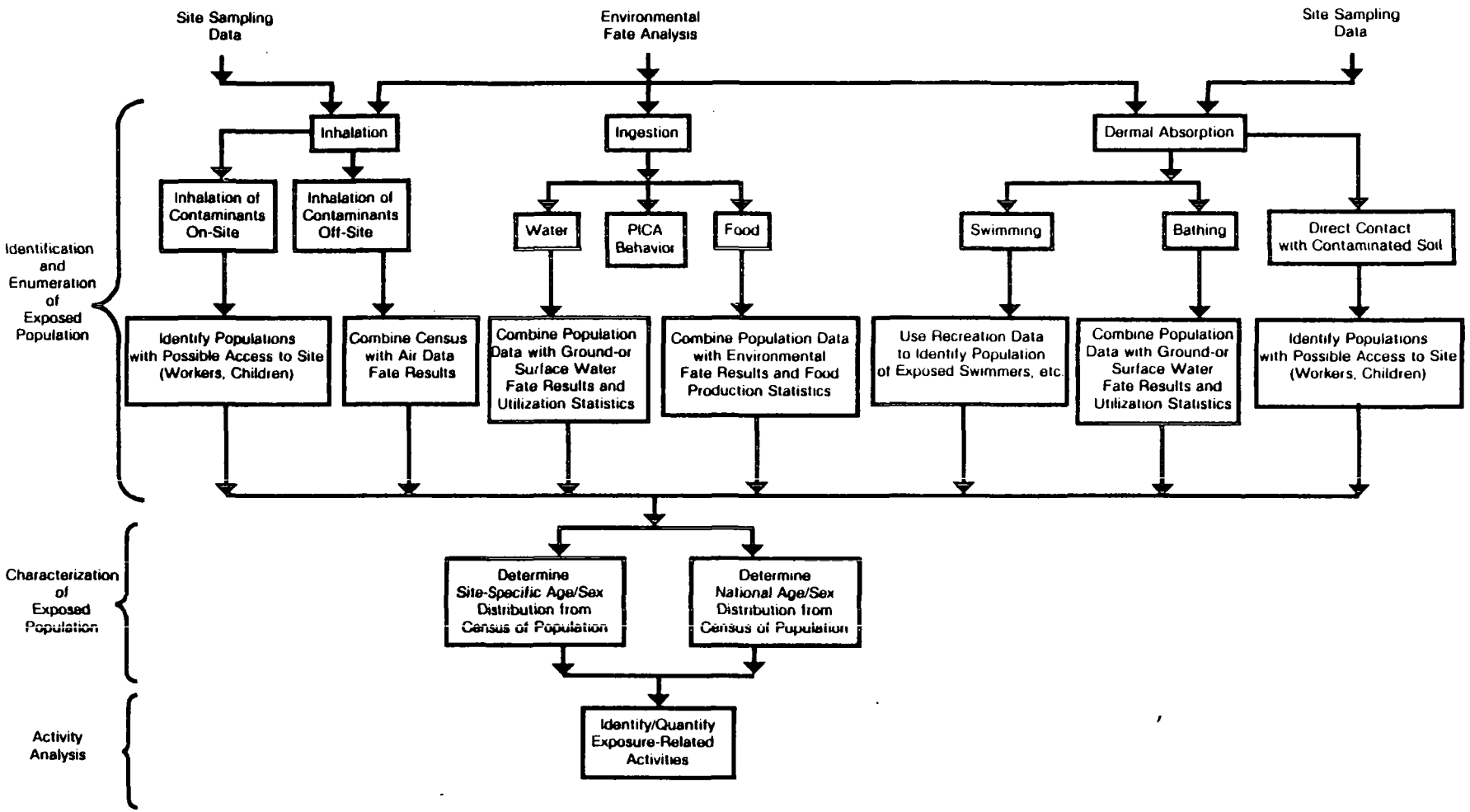
- Persons with a genetic predisposition to certain health effects;
- Persons whose health or resistance to disease is impaired by behavioral factors such as smoking, use of alcohol or drugs, etc;
- Infants, children, and the elderly, who are more susceptible to health impacts from a given exposure than are persons of other ages;
- Persons who are already suffering from disease and may be more susceptible to further impairment as a result of a given level of exposure than are healthy persons;
- Persons who are exposed to naturally high background levels of contaminants (e.g., selenium or arsenic) and may be at greater risk to small incremental increases of hazardous substances than are persons who are not exposed to such background levels; and
- Nutritionally deficient populations who may be less resistant to exposure than those with adequate diet.

While most studies will consider only the exposed population as a whole and not as separate discrete subpopulations, in certain cases, such detailed population analysis may be warranted for in-depth studies.

Age and sex influence the average inhalation rate, the rate of food and water intake, the body area subject to dermal exposure, and the types of food consumed, all of which can affect the level of exposure actually experienced. Some quantitative assessments may require further characterization of populations to determine age- and sex-specific exposure factors.

The third step is activity analysis. Once population identification and characterization have answered the question "Who may be exposed?", the question "How and to what level are component portions of this population exposed?" may next be asked in order to refine the evaluation. This refinement involves determining the exposed population's activities. Comprehensive analysis can encompass the range of indoor, outdoor, and in-car activities. For Superfund Feasibility Studies, however, average values for activity-related considerations usually suffice.

Figure A-2. Quantitative exposed population analysis



The activity analysis can also help to identify high-risk groups. For example, those groups that may experience a significantly higher frequency or duration of exposure as compared with the general population can also be considered high-risk groups.

1.4 Identification and Enumeration of Exposed Human Populations

The major population data base that can be accessed to determine the size, distribution, and demographic characteristics of a geographically defined population is the Census of Population.

The data collected in the Census are organized according to geographic areas. Within these areas, data are further broken down into Census-defined statistical areas and government units. Population data are available within Standard Metropolitan Statistical Areas (SMSAs) down to the level of the "block" and in non-SMSAs to the level of the Enumeration District (ED).

These data are especially useful in quantifying and characterizing populations exposed as a result of their presence in a specific locale (e.g., those exposed to toxics in ambient air or soil). An isopleth map of varying concentrations around a source can be overlaid with Census maps. Such maps are available for areas within SMSAs and can be purchased from the Bureau of the Census. Also, Census Tracts (Series PHC80-2) contains detailed characteristics of the population (e.g., age, sex, race, education) within each tract, a division of an SMSA containing 4,000 residents each. Census Tracts is currently available on microfiche by SMSA and on computer tape.

Many Superfund sites are not within SMSAs. Census data for non-SMSA areas are not available on maps, but can be transcribed from Census publications.

The most useful Census publications for this type of data are *Number of Inhabitants* (Series PC80-1-A) and *General Population Characteristics* (Series PC80-1-B). Each series is currently available and consists of a separate volume for each state, together with a national summary volume. *Number of Inhabitants* provides only population counts, with no demographic data. It provides data down to the level of county subdivision and incorporated town. *General Population Characteristics* provides population counts by age, sex, and other demographic data, and contains data down to the level of small towns (1,000 or more inhabitants).

All printed Census information is available for purchase through the Government Printing Office (GPO); all series issued on microfiche, maps, computer tapes, and technical documentation are available directly from the Customer Services Branch at the Bureau of the Census, Department of Commerce, Washington, D.C., and can be ordered by calling (202) 763-4100. Alternatively, it may be more convenient to contact one of the Census Bureau regional offices. Cities where such offices are located and phone numbers for the public information service within each regional office are listed in Table A-1.

Table A-1. Regional Census Bureau Offices

Atlanta, Ga.	(404) 881-2274
Boston,Mass.	(617)223-0226
Charlotte, N.C.	(704)371-6144
Chicago,Ill.	(312)353-0980
Dallas,Tex.	(214)767-0625
Denver,Colo.	(303)234-5825
Detroit,Mich.	(313)226-4675
KansasCity, Kans.	(913)236-3731
LosAngeles, Calif.	(213)209-6612
NewYork, N.Y.	(212)264-4730
Philadelphia, Pa.	(215)597-8313
Seattle, Wash.	(206)442-7080

1.4.1 Populations Exposed through Air

A convenient means of accessing quantitative population data for a specific area impacted by air contaminants is to directly link environmental fate and exposed populations analysis through use of an integrated computer-based fate model and population data retrieval program called ATM-SECPOP. Developed by the EPA Office of Toxic Substances, Exposure Evaluation Division (OTS-EED), this model primarily analyzes point source emissions, but can also be adapted to area or line source analyses. ATM-SECPOP integrates the output of a concentration prediction model (ATM) (Patterson et al. 1982); a population distribution data base (the proprietary 1980 Census Master Area Reference File (MARF)), which is accessed via a population distribution model called SECPOP; and graphic and mapping information displays. This integration affords a rapid and efficient means of generating and presenting exposure data relating to the airborne release of chemical substances. The graphic display functions can be used to illustrate the relationship of variables such as the distribution of exposure or concentration versus distance for any or all directions around a facility. Graphic displays may be in the form of bar charts, scatter plots, rose diagrams, or maps. Because of the proprietary nature of the data contained in MARF, ATM-SECPOP's use is restricted to personnel and contractors of EPA, Office of Toxic Substances (EPA-OTS). Special arrangements can be made for others to use the data. Inquiries should be directed to the Modeling

Section of the Exposure Assessment Branch of EPA-OTS in Washington, D.C. A detailed discussion of ATM is presented in Chapter 3 of this manual.

Where sites are accessible, the possibility that children may enter and explore or play on the site should be evaluated. On-site, children may experience inhalation exposure to contaminated dust, volatiles, or both. In some cases, the site boundary may adjoin residential properties, and the area of contamination may actually include such residences. Accurate estimation of the potentially exposed population in such a case is difficult; it can be assumed that each household with children in the immediate vicinity of the site has one child who may find the site inviting. This should provide an upper bound estimate on the actual number of children who may enter the site. The Bureau of the Census (1986) reports that in 1984, 50.1 percent of all U.S. households included children. This percentage can be applied to the total number of local households to enumerate those in the area with children. The analyst must decide which households are close enough to the site to be considered.

Similarly, workers conducting activities at the site may also experience inhalation exposure. Local authorities (e.g., Zoning Board) may be able to supply information on the likelihood of on-site work-related activities that can be used to estimate the number of workers who may become exposed. Remediation workers are not included in this estimated exposed population.

1.4.2 Populations Exposed through Surface Water or Ground Water

Environmental fate analysis results can be used to identify geographically-defined sources of recreational (aquatic) dermal exposure, such as river reaches downstream of an uncontrolled hazardous site. The exposed population comprises swimmers in those specific contaminated waters. The local government agency concerned with recreation should be able to provide estimates of the populations swimming in local waters; this will usually be the state, city, or county Department of Parks or Recreation. Alternatively, one can use the following national average value from the Bureau of Outdoor Recreation (USDOI 1973): 34 percent of the total population swims outdoors in natural surface waterbodies (including oceans, lakes, creeks, and rivers).

All persons served by a water supply system that draws water from a contaminated water source must be considered as potentially exposed through ingestion and dermal exposure while bathing. Information concerning local surface drinking water sources and populations served can be obtained from the local Department of Public Works, Planning Department, or Health Department. These sources should be able to provide information on public departments or private drinking water treatment companies that use ground water as their raw water supply, and also on the number of households drawing water from private wells.

1.4.3 Populations Exposed through Food

Exposure to contaminated food will usually be associated with fruit and vegetables grown in home gardens or with game residing in or using contaminated areas. In order to identify the number of persons consuming contaminated home grown fruit and vegetables, first consult General Population Characteristics, Series PC80-1-B, to learn the total number of households in a given geographic area. Then the data presented in Table A-2, which provide estimates of the percent of households in urban and rural areas that have fruit and vegetable gardens and the average number of persons per household, can be applied to the local population data to estimate the number of persons likely to consume contaminated home grown produce.

The USDA *Food Consumption of Households* report series can be consulted to estimate the local population using a given food item for urban, rural non-farm, and rural farm locales. These reports present seasonal food use survey data on the following bases: Northeast (USDA 1983a), North Central (USDA 1983b), South (USDA 1983c), and West (USDA 1983d). More aggregated data are also provided for the entire United States in a companion report (USDA 1983e). The percent of households using a given food item can be obtained from these reports. The product of this value and the total resident population of an area is an estimate of the local exposed population. Similar national level data are also provided on the basis of age and sex in *Food and Nutrient Intakes of Individuals in 1 Day in the United States* (USDA 1980). In addition, the U.S. Food and Drug Administration (FDA) can be contacted for data concerning daily intakes of various food items. Such data have been compiled for the FDA Total Diet Study (Pennington 1983).

Table A-2. U.S. Home Fruit and Vegetable Garden Use, 1977

Urbanization	Percent of households with gardens	Household size (no. of persons)	Percent of total U.S. population
Urban	43	3.17	32
Rural non-farm	41	3.44	9
Rural farm	84	3.86	3

Source: USEPA 1980.

Monitoring data may indicate whether fish and game are contaminated in the subject area. One can estimate the fishing population by contacting the local agency responsible for issuing fishing licenses; this may be the state fish and game commission or the state department of natural resources. Since there are 2.69 persons in the average household (Bureau of the Census 1986), one can estimate the actual exposed population by multiplying 2.69 by the number of licensed hunters or fishermen in the area.

1.4.4 Populations Exposed through Soil

Exposure to contaminated soil constitutes a potential exposure route for workers or children playing outdoors. Neighborhood children playing at the site can be exposed to high levels of contaminants. Soil-related exposure in such cases would be through direct dermal contact with the contaminated soil. Another potentially significant, but infrequently encountered, exposure mechanism involves children who eat dirt; this eating behavior, known as pica, may lead to their actually ingesting contaminated soil. Hand-to-mouth contact during normal play is a more common means of ingesting soil, however. For any site located near residential areas, the degree of accessibility to children should be considered. Bureau of the Census data can be used as described in Section A-1.4.1 to estimate the number of local children who may have access to the site.

In addition, workers conducting activities at the site (other than remediation) may have direct dermal contact with contaminated soils. Section A-1.4.1 provides general guidance to identify and enumerate exposed worker populations.

1.5 Population Characterization

After exposed populations have been identified and enumerated, they can be characterized by age and sex factors. The physiological parameters that determine the dose received per a given level of exposure (e.g., breathing rate, skin surface area, and ingestion rate) are often age- or sex-specific. Also, from a toxicity standpoint, subpopulations defined by age or sex, such as the elderly or women of childbearing age, may be especially susceptible to a chemical substance. Superfund studies will generally use average values, but by characterizing exposed populations, one can determine exposure distributions within the population at large and delineate specific high-risk subpopulations.

The Census Publication series *General Population Characteristics* (PC80-1-B) cites figures for the age and sex structure of the population residing in a specific area. Separate volumes for each state contain age and sex breakdowns at the level of county subdivisions and small towns. If more detail is required, the Census Bureau microfiches containing this information at the Census tract level (only available by SMSAs).

In the case of exposure resulting from ingestion of food, the food consumption surveys of the USDA (1983a-e) record age and sex data for the sampled population. These data are contained in five separate regional reports; the appropriate one should be consulted.

In lieu of obtaining site-specific data, one can use the population characteristics of the U.S. as a whole, provided in the yearly Statistical Abstract of the United States (for example, see Bureau of the Census 1986), to approximate the population distribution in the area of concern.

1.6 Activity Analysis

Activities engaged in by members of a given population or subpopulation can dramatically affect the level of human exposure to environmental contaminants. For example, persons whose lifestyle or employment involves frequent strenuous activity will inhale larger volumes of air per unit time than will those living a less strenuous life, and will experience a higher level of exposure to airborne contaminants.

Activity analysis allows refinement of certain parameters used in the calculation of exposure, including:

- Inhalation rate;
- Frequency of exposure; and
- Duration of exposure.

The procedure for integrating activity-related inhalation, frequency, and duration data into the exposure assessment process is detailed in the following chapter.

Chapter 2
Exposure Calculation and Integration

This chapter provides guidance for calculating and integrating exposures to all populations affected by the various exposure routes associated with a given uncontrolled hazardous waste site. Specifically, guidance is provided to estimate exposure from:

1. Inhalation
   a. Ambient air
   b. Indoor air (contaminants released during showering)

2. Dermal contact
   a. Water (swimming)
   b. Soil

3. Ingestion
   a. Food
   b. Water
   c. Soil

This analysis is based on the results of all previous analyses, and is the final stage of the exposure assessment. This guidance is complete; no additional documentation is required to finish the analysis.

Integrated exposure analysis is conducted for only those contaminants having complete exposure pathways (i.e., those contaminants that are released and migrate from the site and that do contact human populations). Therefore, no screening evaluation is included in the exposure integration process. While calculating the exposure incurred is traditionally the final step in the quantitative exposure assessment process, it can also be viewed as a component of the human health risk assessment. Therefore, the material detailed in this chapter is also discussed in the Superfund Public Health Evaluation Manual (USEPA 1985).

Exposure is defined as the amount of pollutant contacting body boundaries (skin, lungs, or gastrointestinal tract). Exposure calculation considers how often populations come into contact with contaminants in specific environmental media, the mode of such contact, and the amount of contaminated medium that contacts the internal or external body surface during each exposure event. The goal of this analysis is to quantify the amount of contaminant contacted within a given time interval.

Short-term and long-term exposures are calculated in the same manner. First, for each exposure scenario under consideration, an exposure per event is estimated. This exposure value quantifies the amount of contaminant contacted during each exposure event, with "event" being defined differently depending on the nature of the scenario under consideration (e.g., each day spent swimming in a contaminated river is a single swimming exposure event, each day's inhalation of contaminated air is an inhalation exposure event). Event-based exposure estimates take into account the concentration of contaminant in the medium through which exposure occurs, the rate of contact with such media (inhalation rate, ingestion rate, etc.), and the duration of each event.

The analyst can convert event-based exposure values to final exposure values by multiplying the exposure per event by the frequency of exposure events over the timeframe being considered. Short-term exposure is based on the number of exposure events that occur during the short-term timeframe (10 to 90 days), while long-term exposures are based on the number of events that occur within an assumed 70-year lifetime. The 70-year assumed average lifetime is traditionally used in exposure assessments, and it provides a conservative upper bound of lifetime exposure. Certain exposure scenarios, however, may only apply to short-term exposure. Whenever practical, the analyst should strive to determine the timeframe over which a given exposure pathway would be expected to affect the exposed population. Once determined, the timeframe will indicate whether that pathway should be evaluated on a short- or a long-term basis.

Exposure estimates are expressed in terms of mass of contaminant/unit of body mass/day by dividing daily exposure by the value for total body mass of an average individual in the exposed population. For Superfund studies, an average adult body mass of 70 kg will usually be adequate for this conversion. In cases where exposure to specified subpopulations must be evaluated, values for other than average

adults may be required. Consult Anderson et al. (1984) to obtain alternative body mass values. Similarly, average values for activity-related parameters (e.g., inhalation rate) generally will be adequate for Superfund site evaluations. For special situations and detailed exposure analysis, analysts can refer to the discussion of activity data in Freed et al. (1985). An exposure factors handbook is currently under development (USEPA 1987), and the analyst performing exposure assessments after publication of this manual should consult that document for the most up-to-date exposure factors.

The following sections address the exposure calculation process specific to each exposure mechanism. Data management forms designed to organize and tabulate the data in the exposure calculation process are presented in Appendix C.

2.1 Inhalation Exposure

Inhalation exposure per event is estimated based on the hours per event, the inhalation rate of the exposed individual during the event, and the concentration of contaminant in the air breathed. The formula for calculating event-based exposure is the following:

$$IEX = t_e \times I \times \bar{C}(X) \times F \div BW \div 2.56 \times 10^4 \frac{\text{days}}{\text{lifetime}} \qquad \text{(A-1)}$$

where

IEX	=	estimated inhalation exposure, (mg/kg/day).
t_e	=	duration of an exposure event, (hours/event).
I	=	average inhalation rate of exposed persons, (m^3/hr).
$\bar{C}(X)$	=	contaminant air concentration throughout the exposure period, (milligrams/m^3).
BW	=	average adult body weight, (70 kg).
F	=	frequency of exposure event, (number/lifetime).

Short-term exposure is calculated using the short-term contaminant air concentration, and long-term exposure is based on the long-term concentration.

Inhalation exposures are keyed to geographic locations delineated during the Environmental Fate Analysis. Ambient concentration is generally assumed to be homogeneous throughout a limited area or sector (within an isopleth); however, this assumption is not always well-founded. Numerous studies have shown that there can be marked differences in indoor and outdoor concentrations of pollutants (Budiansky 1980, Moschandreas et al. 1978) or among microenvironments in the same area (Ott 1981). To account for these differences when calculating exposure, several investigations have coined the term "microenvironment," which refers to a type of physical setting where concentrations of pollutants can be expected to be similar. For Superfund studies, it is usually unnecessary to disaggregate analysis on a microenvironment basis. Instead, it can generally be assumed that contaminants have been present long enough for indoor-to-outdoor concentrations to have reached equilibrium.

To calculate exposure duration, the analyst considers the amount of time exposed persons actually spend in the contaminated area. For example, if a site is in a residential area, one can conservatively estimate exposure by assuming that all residents spend the entire 24-hour day within the contaminated zone. If a site is located in an industrialized area, it may be more appropriate to base duration on an 8-hour workday, if it can be reasonably assumed that workers do not also live in the immediate industrialized area. Such factors must be evaluated on a case-by-case basis. For inhalation exposure, frequency is assumed to be daily.

For a general application, use an average adult value for inhalation rate. An example of an adult average derived from experimental results (USEPA 1981) is an inhalation rate of 1 m^3/hour. This value can be used to conservatively estimate exposure regardless of microenvironments or activity.

Generating time-weighted average inhalation rates provides a more precise estimate of inhalation rate. This calculation is based on microenvironment-related data and activity stress levels/ventilation rates associated with the individual microenvironment. If this level of detail is warranted, the inhalation rates presented in Table A-3 can be used. Freed et al. (1985) cite directions for developing time-weighted average inhalation rates.

To calculate ambient inhalation exposure, one should obtain contaminant air concentration values from the results of the environmental fate analysis. In one case, however, concentration values will have to be calculated in the exposure integration stage of the exposure assessment. Persons showering or bathing in potable water contaminated with toxics may be exposed through inhalation if the contaminants are volatile. This is especially true of showering, since the high turbulence, combined with the elevated temperature of the shower water, can produce a significant release of volatile components.

Various approaches are available to estimate contaminant concentrations indoors. These approaches depend on a number of factors, including the room air volume, air exchange and mixing factors, contaminant concentration in the water, the amount of water used, and the manner in which a contaminant

Table A-3. Summary of Human Inhalation Rates for Men, Women and Children by Activity Level (m^3/hour)[a]

	Resting[b]	Light[c]	Moderate[d]	Heavy[e]
Adult male	0.6	1.3	2.8	7.1
Adult female	0.6	1.3	2.4	4.9
Average adult[f]	0.6	1.3	2.6	6.0
Child, age 6	0.4	1.4	2.1	2.4
Child, age 10	0.4	1.7	3.3	4.2

[a]Values of inhalation rates for males, females, and children presented in this table represent the midpoint of ranges of values reported for each activity level in Anderson et al. (1984)
[b]Includes watching television, reading, and sleeping.
[c]Includes most domestic work, attending to personal needs and care, hobbies, and conducting minor indoor repairs and home improvements.
[d]Includes heavy indoor cleanup and performance of major indoor repairs and alterations and climbing stairs.
[e]Includes vigorous physical exercise and climbing stairs carrying a load.
[f]Derived by taking the mean of the adult male and adult female values for each activity level. A representative 24-hour breathing rate for an average adult is 1.1 m^3/hour. This value is based on the assumption that the average adult spends 93.2 percent of the time at the light/resting level of activity, 5.8 percent at a moderate level of activity, and 0.9 percent at a heavy level of activity. Values for the percent of time spent at each activity level are from Freed et al. (1985).

is released into room air (instantaneously, continuously, time-dependent). If showering/bathing exposure estimation is required for a Superfund exposure assessment, the analyst is referred to Versar (1984) for a detailed discussion of techniques to estimate indoor air contaminant concentration. For both showers and baths, the analyst should assume a continuous contaminant release during the bathing/showering period. Values for the other variable factors mentioned above can be obtained from Versar (1985).

To evaluate inhalation exposure to contaminants volatilizing from potable water while showering, the analyst should again assume frequency to be daily. Each shower is assumed to last 15 minutes.

Inhalation exposure to swimmers can be based on monitored or estimated ambient air concentrations above a contaminated water body. To estimate concentrations, calculate the rate of volatilization of the contaminant from the water body and use this value as the input to a "box model" air migration model. The dynamic release rate can be calculated using Equations 2-10, 2-15, 2-16, and 2-17. The recommended air model is BOXMOD (in EPA's GEMS system, see Chapter 3).

2.2 Dermal Exposure

Dermal exposure is determined by the concentration of hazardous substance in a contaminated medium that is contacted, the extent of contact (i.e., the body surface area contacted), and the duration of such contact. For exposure to contaminated water, dermal exposure per event is calculated as follows:

$$DEX = t_e \times AV \times C \times PC \times F \times 1 \text{ liter}/1000 \text{ cm}^3 \div BW \div 2.56 \times 10^4 \frac{\text{days}}{\text{lifetime}} \quad \text{(A-2)}$$

where

DEX	=	estimated dermal exposure, (mg/kg/day).
t_e	=	duration of exposure, (hours/event).
AV	=	skin surface area available for contact, (cm^2).
C	=	contaminant concentration in water, (mg/liter).
PC	=	dermal permeability constant for the subject contaminant, (cm/hr).
F	=	frequency of exposure events per lifetime.
BW	=	average adult body weight, (70 kg).

The term 1 liter/1,000 cm^3 is a volumetric conversion constant for water.

When possible, it is important to consider the degree to which a given contaminant is actually able to enter the body. Some compounds will not readily penetrate the skin, while others may do so at a rapid rate. The above equation can only be used in cases where dermal permeability constants for the contaminant(s) of concern are known. Table A-4 lists dermal permeability constants for selected compounds. For many compounds, however, dermal permeability constants will not be available. In such cases, the analyst must assume that contaminants are carried through the skin as a solute in water which is absorbed (rather than being preferentially absorbed independently of the water), and that the contaminant concentration in the water being absorbed is equal to the ambient concentration. Thus, the permeation rate of water across the skin boundary is assumed to be the factor controlling the contaminant absorption rate. Short-term dermal exposure per event is calculated using the short-term contaminant concentrations in water or soil, and long-term exposure is based on the long-term contaminant concentrations.

The local recreation department may have detailed data quantifying the duration and frequency of water use for swimming. When such locale-specific data are not available, the following national average figures, based on data from the Bureau of Outdoor Recreation (USDOI 1973), can be applied:

- Frequency of exposure = 7 days/year.

Table A-4. Permeability Constants for Various Compounds

Compound	Permeability constant[a] (cm/hr)	Reference
SURFACTANTS		
Decanoic acid	1.00E-03	Howes 1975
Dodecanoic acid	2.00E-03	Howes 1975
Tetradecanoic acid	6.00E-04	Howes 1975
Hexadecanoic acid	1.20E-05	Howes 1975
Octadecanoic acid	6.00E-06	Howes 1975
Sodium dodecyl sulfate	2.00E-03	Howes 1975
Sodium dodecyl isothionate	5.40E-05	Howes 1975
Sodium p-1-dodecyl benzenesulphonate	6.00E-06	Howes 1975
Sodium laurate	1.00E-03	Tregear 1966
IONS		
Aluminum	7.20E-06	Tregear 1966
Potassium	6.70E-05	Tregear 1966
Bromide	1.80E-05	Tregear 1966
Palmitate	4.20E-05	Tregear 1966
Laurate	3.00E-03	Tregear 1966
DRUGS		
Methotrexate	6.00E-10	McCullough et al. 1976
Benzoyl peroxide	5.10E-07	Nacht et al. 1981
Estradiol	3.90E-03	Galey et al. 1976
Amphetamine	1.40E-05	Galey et al. 1976
Ouabain	3.90E-06	Sutton 1973
Burimamide	1.70E-07	Sutton 1973
Metiamide	1.10E-07	Sutton 1973
Cimetidine	3.30E-07	Sutton 1973
PHENOLS		
Resorcinol	2.40E-03	Roberts et al. 1977
p-Nitrophenol	5.58E-02	Roberts et al. 1977
n-Nitrophenol	5.58E-02	Roberts et al. 1977
Phenol	8.22E-02	Roberts et al. 1977
Methylhydroxybenzoate	9.12E-02	Roberts et al. 1977
n-Cresol	1.52E-01	Roberts et al. 1977
o-Cresol	1.57E-01	Roberts et al. 1977
p-Cresol	1.75E-01	Roberts et al. 1977
beta-Naphthol	2.79E-01	Roberts et al. 1977
o-Chlorophenol	3.31E-01	Roberts et al. 1977
p-Ethylphenol	3.49E-01	Roberts et al. 1977
3,4-Xylenol	3.60E-01	Roberts et al. 1977
p-Bromophenol	3.60E-01	Roberts et al. 1977
p-Chlorophenol	3.60E-01	Roberts et al. 1977
Thymol	5.28E-01	Roberts et al. 1977
Chlorocresol	5.50E-01	Roberts et al. 1977

(Continued)

Table A-4. (Continued)

Compound	Permeability constant[a] (cm/hr)	Reference
PHENOLS (Continued)		
Chloroxylenol	5.90E-01	Roberts et al. 1977
1,4,6-Trichlorophenol	5.94E-01	Roberts et al. 1977
2,4-Dichlorophenol	6.01E-01	Roberts et al. 1977
STEROIDS		
Progesterone	1.50E-03	Scheuplein et al. 1969
Pregnenolone	1.50E-03	Scheuplein et al. 1969
Hydroxypregnenolone	6.00E-04	Scheuplein et al. 1969
Hydroxyprogesterone	6.00E-04	Scheuplein et al. 1969
Cortexone	4.50E-04	Scheuplein et al. 1969
Testosterone	4.00E-04	Scheuplein et al. 1969
Cortexolone	7.50E-05	Scheuplein et al. 1969
Corticosterone	6.00E-05	Scheuplein et al. 1969
Cortisone	1.00E-05	Scheuplein et al. 1969
Hydrocortisone	3.00E-06	Scheuplein et al. 1969
Aldosterone	3.00E-06	Scheuplein et al. 1969
Estrone	3.60E-03	Scheuplein et al. 1969
Estradiol	3.00E-04	Scheuplein et al. 1969
Estriol	4.00E-05	Scheuplein et al. 1969
Dihydroepiandrosterone[b]	1.70E-04	Schaefer et al. 1982
Dihydrotestosterone[b]	3.90E-04	Schaefer et al. 1982
ALCOHOLS		
Methanol	5.00E-04	Scheuplein and Blank 1971
Ethanol	8.00E-04	Scheuplein and Blank 1971
Propanol	1.20E-03	Scheuplein and Blank 1971
Butanol	2.50E-03	Scheuplein and Blank 1971
Pentanol	6.00E-03	Scheuplein and Blank 1971
Hexanol	1.30E-02	Scheuplein and Blank 1971
Heptanol	3.20E-02	Scheuplein and Blank 1971
Octanol	5.20E-02	Scheuplein and Blank 1971
Nonanol	6.00E-02	Scheuplein and Blank 1971
Decanol	8.00E-02	Scheuplein and Blank 1971
GLYCOL ETHERS		
2-Methoxyethanol	2.89E-03	Dugard et al. 1984
2-Ethoxyethanol	8.42E-04	Dugard et al. 1984
2-Ethoxyethanol acetate	8.07E-04	Dugard et al. 1984
2-n-Butoxyethanol	2.14E-04	Dugard et al. 1984
1-Methoxypropan-2-ol	1.25E-03	Dugard et al. 1984
2-(2-Methoxyethoxy)ethanol	2.06E-04	Dugard et al. 1984
2-(2-Ethoxyethoxy)ethanol	1.32E-04	Dugard et al. 1984
2-(2-n-Butoxyethoxy)ethanol	3.60E-05	Dugard et al. 1984

(Continued)

Table A-4. (Continued)

Compound	Permeability constant[a] (cm/hr)	Reference
PESTICIDES[c]		
Azodrin	9.80E-04	Feldman and Maibach 1974
Ethion	2.20E-04	Feldman and Maibach 1974
Guthion	1.06E-03	Feldman and Maibach 1974
Malathion	5.50E-04	Feldman and Maibach 1974
Parathion	6.50E-04	Feldman and Maibach 1974
Baygon	1.31E-03	Feldman and Maibach 1974
Carbaryl	4.90E-03	Feldman and Maibach 1974
Aldrin	5.20E-04	Feldman and Maibach 1974
Dieldrin	5.10E-04	Feldman and Maibach 1974
Lindane	6.20E-04	Feldman and Maibach 1974
2,4-D	3.90E-04	Feldman and Maibach 1974
Diquat	2.00E-05	Feldman and Maibach 1974
OTHER		
Water	8.00E-04	Blank et al. 1984
Ethylbenzene	1.00E-03	Dutiewicz and Tyras 1967
Styrene	6.00E-04	Dutiewicz and Tyras 1968
Toluene	9.00E-04	Dutiewicz and Tyras 1968
Aniline[b]	2.00E-02	Baranowska-Dutkiewicz 1982
N-nitrosodiethanolamine	5.50E-05	Bronaugh et al. 1981
Ethyl ether	1.70E+01	Scheuplein and Blank 1971
2-Butanone	5.00E+00	Scheuplein and Blank 1971
1-Butanol	4.00E+00	Scheuplein and Blank 1971
2-Ethoxyethanol	3.00E-01	Scheuplein and Blank 1971
2,3-Butanediol	5.00E-02	Scheuplein and Blank 1971
Benzene[b]	4.10E-01	Baranowska-Dutkiewicz 1982
Desoximetasone[b,d]	3.40E-05	Schaefer et al. 1982
Linoleic acid[b,d]	1.60E-05	Schaefer et al. 1982
Dithranol[b]	2.10E-04	Schaefer et al. 1982
Theophylline[b]	2.50E-05	Schaefer et al. 1982
Caffeine[b]	3.30E-04	Schaefer et al. 1982
8-Methoxypsoralen[b,d]	9.90E-04	Schaefer et al. 1982
p-Butoxyphenylacethydroxamic acid[b,d]	9.80E-05	Schaefer et al. 1982
Triacetoxyanthracene[b]	5.80E-05	Schaefer et al. 1982
Heparin[b,d]	8.20E-05	Schaefer et al. 1982
Carbon disulfide[b]	5.50E-02	Baranowska-Dutkiewicz 1982

[a] Permeability constants are for contaminants as a dilute solution in water, except as noted.
[b] Calculated permeability constant, subject to error.
[c] Permeability constants are for contaminants in acetone. These values should not be used for dermal exposure due to contact with contaminated water. These values should be used for dermal exposure to pure wastes.
[d] Permeability constants are for contaminants in gel. These values should not be used for dermal exposure due to contact with contaminated water. These values may be used for dermal exposure to pure wastes.

- Duration of exposure = 2.6 hours/day.

Dermal absorption of waterborne contaminants may be a significant exposure route. The factors that influence dermal absorption of chemicals are: (1) the nature of the compound (molecular weight, lipophilicity), (2) the presence of other compounds that might facilitate passage of a chemical though the skin (e.g., chelating or complexing agents), and (3) the permeability of the skin. Generally only lipid-soluble, non-ionized compounds are absorbed significantly through the skin. Also, the skin is normally permeable only to compounds whose molecular weights are less than 500 Daltons. The permeability of the skin to larger molecular weight compounds and to less lipophilic compounds can be increased when corrosive agents such as acids are present or when there are skin abrasions. For waterborne chemicals, exposure through the skin is almost directly proportional to concentration.

Brown, Bishop, and Rowan (1984) recently reported that when compared with ingestion, dermal absorption of volatile organic contaminants in drinking water accounted for approximately 29 to 91 percent of the total dose incurred, with the average being about 64 percent. The dermal exposure route becomes especially pertinent when organic contaminants are present in very dilute aqueous solution, as may often be the case at Superfund sites. In certain cases, then, dermal exposure to contaminants contained in ground or surface water may actually overshadow ingestion exposure.

When persons become exposed to contaminants in drinking water, the dermal exposure associated with bathing or showering should also be considered. One can use the same approach to assess bathing/showering as was used for swimming. Generally, an average frequency of one bath or shower per day can be assumed, and each event can be estimated to last 15 minutes.

For swimming or bathing exposure, the surface area available for dermal exposure is assumed to equal the total amount of human skin surface area. Average availability values are given below for adults and children. If the exposed population is not separated by age groups, both availability values should be used to represent a general range of exposure for the total swimming or bathing population. Both availability figures cited below are taken from Anderson et al. (1984):

- Average adult (male and female, 20-30 yrs) = 18,150 cm^2.

- Average child (male and female, 3-12 yrs) = 9,400 cm^2.

Direct dermal contact with contaminants present in soil is calculated as follows:

$$DEX = C_i \times AV \times DA \times F \div BW \div 2.56 \times 10^4 \frac{\text{days}}{\text{lifetime}} \qquad \text{(A-3)}$$

where

DEX	=	dermal exposure, (mg/kg/day).
C_i	=	weight fraction of chemical substance in soil, (unitless).
AV	=	skin surface area available for contact, (cm^2).
DA	=	dust adherence, (mg/cm^2).
F	=	frequency of exposure events per lifetime.
BW	=	average adult body weight, (70 kg).

Values for contaminant weight fraction in the contaminated soil will be available from the site survey. Skin surface availability depends on the nature of activity being conducted, and can vary for a given activity depending on the season of the year. Anderson et al. (1984) provide data on skin surface areas of different parts of the body for adults and children. Based on a projection of the type of activity at the site and the age of the exposed population (i.e., workers or children), the data in Anderson et al. can be used to develop skin surface estimates for use in estimating direct dermal exposure.

Data on dust adherence to skin (DA) are limited, although the following experimental values for (soil-related) dust adherence were reported by the Toxic Substance Control Commission of the State of Michigan (Harger 1979):

- Commercial potting soil adheres to hands at 1.45 mg/cm^2.

- Dust of the clay mineral kaolin adheres to hands at 2.77 mg/cm^2.

The degree to which these values represent dust adherence at any given site is uncertain, as such adherence will depend on a variety of site-specific factors. Therefore, instead of selecting one of the above values to estimate direct dermal exposure, it is suggested that the analyst use both values and generate an exposure range. The lifetime frequency of direct dermal exposure will also vary considerably and will depend on the nature of the site, its ease of access, and a variety of other factors. Thus, contact frequency should be estimated on a case-by-case basis, based on knowledge of the site and its environs.

Note that this approach is conservative in that it assumes that all of the contaminant adsorbed to the soil (dust) particles is available for absorption through the skin. In fact, only a percentage of the total adsorbed contaminant mass may actually be available for such absorption, as some percentage may remain bound to the soil particle.

The site survey will provide values for the contaminant weight fraction in the contaminated soil. Skin surface availability depends on the nature of the activity being conducted, and can vary for a given activity depending on the season of the year. Anderson et al. (1984) provide data on skin surface areas of different parts of the body for adults and children. Based on a projection of the type of activity at the site and the age of the exposed population (i.e., workers or children), one can use the data in Anderson et al. to develop skin surface estimates for use in estimating direct dermal exposure.

The lifetime frequency of direct dermal exposure will vary considerably and will depend on the nature of the site, its ease of access, and other factors. Contact frequency should be estimated on a case-by-case basis, based on knowledge of the site and its environs.

2.3 Ingestion Exposure

2.3.1 Food/Soil

Food ingestion exposure is estimated as the product of contaminant concentration in the food consumed and the amount of food consumed per day. Frequency is daily for foods that are a regular part of the diet. For recreationally caught fish, frequency can be estimated based on the seasonal nature of fishing involved.

USDA source materials listed in Section A-1.4.3 are also useful in quantifying the amount of contaminated food ingested. The *Food Consumption of Households* report series provides data quantifying the amount of various food categories consumed by households on a seasonal basis. Similar data are presented in *Food and Nutrient Intakes of Individuals in 1 Day in the United States*. The first source can be used to derive estimates of the amount of various foods consumed by the overall exposed population by applying seasonal percentage use values to local population census data. The second source is used in subpopulation analyses by applying sex- and age-specific consumption values to census data for the exposed population.

Consumption of fish caught in contaminated waters may be an important ingestion route, since certain contaminants of concern tend to biomagnify in the food chain. This phenomenon results in tissue concentrations of contaminants in predator fish exhibiting levels that greatly exceed the ambient concentration in the waterbody. An average daily fish ingestion rate for the U.S. population has been estimated as 6.5 grams per day (USEPA 1980b). Persons for whom fish constitutes a major portion of the overall diet may consume up to 124 grams per day (USDA 1980). A West Coast study of consumption of fish caught in contaminated waters by sport fishermen (Puffer et al. 1981) reports a median fish ingestion rate of 37 grams/day. This report also lists a maximum rate of 225 grams/day.

Ingestion exposure estimates are calculated in the same manner, regardless of the type of food ingested. Multiplication of the contaminant concentration in the ingested food by the amount of contaminated food ingested per day yields exposure per day.

Children may ingest soil during play both inadvertently and intentionally (pica behavior). In those assessments where the exposed populations analysis has found that children may have access to areas of contaminated soil, this exposure route should be evaluated. Data quantifying the amount of soil ingested by children are conflicting and vary considerably. For example, Calabrese et al. (1987) report that estimates range from a low of 10 mg/day (for 2-year-old children) to a high of 10,000 mg/day (for 1.5- to 3.5-year-old children). Within this range, reasonable typical values can be identified and associated with various age groups, if desired. For studies warranting such detail, the daily soil ingestion rate values presented in Table A-5 can be used. For studies that do not require such detail, one can use an overall average soil ingestion value of 100 mg/day.

Table A-5. Typical Daily Soil Ingestion Rates for Children by Age Group

Age	Soil ingestion range (mg/day)
0-9 months	0
9-18 months	50
1.5 - 3.5 years	200
3.5 - 5 years	50
5 - 18 years	10

Source: Calabrese et al. 1987.

2.3.2 Water

Event-based water ingestion exposure equals the daily total amount of contaminant ingested from either surface or ground waters affected by the Superfund site. This exposure is determined by the contaminant concentration in the water and the amount of water ingested per day. On average, an adult ingestion coefficient of 2.0 liters per day (USEPA 1980b) can be used for Superfund site analyses. Frequency of drinking water exposure is daily.

When contaminated surface waters are used recreationally, it may be appropriate to estimate exposure that results from inadvertently ingesting contaminated water while swimming. For this analysis, the same values for event frequency and duration previously presented in Section A-2.2 should be used. In addition, to estimate the amount of contaminated water ingested per event, an assumed value of 50 ml per hour can be used.

2.4 Exposure Integration

The final step in the exposure assessment process for uncontrolled hazardous waste sites is the integration of all exposures experienced by individual exposed populations. This simply involves organizing the results of the previous analyses to total all exposures to a given hazardous substance experienced by each population segment. Because different chemicals exhibit different toxicological properties, exposures to each contaminant of concern are considered separately. Note that in some cases, individual populations may be exposed to a given chemical in a particular medium through more than one exposure scenario. For example, persons who swim in contaminated waters may obtain their drinking water from the same contaminated waterbody. In such cases, the dermal exposure experienced while swimming can be added to that experienced during bathing or showering to generate an overall dermal exposure value for that population segment. The data management forms supplied in Appendix C are designed to help organize the results of exposure calculation and integration.

Chapter 3
Appendix A References

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Appendix B

Possible Exposure Assessment Data Requirements for Uncontrolled Hazardous Waste Sites and Index to Variable Terms

Table B-1. Possible Data Requirements for Estimation of Contaminant Release and Transport and Exposed Populations

Type of Analysis	Type of Site	Area of Concern	Area Subclass	Parameter
Contaminant release	Contaminated surface soil (includes spills and leaks)	Particulate release	Wind erosion	• Soil erodibility index[a] • Soil ridge roughness factor[a] • Field length along prevailing wind direction • Vegetative cover factor • Concentrations of contaminants[b] • Volume of contaminated region[b]
			Unpaved roads	• Silt content • Mean speed of vehicles traversing contaminated area[d] • Mean weight of vehicles traversing contaminated area[d] • Mean number of wheels of vehicles traversing contaminated area[d]
			Excavation and transfer of soil	• Silt content[c] • Mean wind speed[e] • Drop height • Material moisture content • Dumping device capacity
		Volatilization	Short-term release	• Vapor concentration of contaminants in soil pore spaces[f]
			Long-term release	• Depth from soil surface to bottom of contaminated region[b] • Area of contamination[b] • Depth of "dry" (uncontaminated) zone at sampling time[b] • Concentrations of contaminants in soil and in liquid phase[b] • Soil porosity[b,c] • Absolute temperature[b,e] • Time measured from sampling time
		Runoff to surface water		• Soil erodibility factor[g] • Slope - length factor • Vegetative cover factor[d] Erosion control practice factor[d] • Area of contamination • Soil bulk density[c] • Total areal concentrations of contaminants
		Release to ground water		- See Chapter 3.6 of Manual

(Continued)

Table B-1. (Continued)

Type of Analysis	Type of Site	Area of Concern	Area Subclass	Parameter
	Landfill	Volatilization	No internal gas generation	• Area of contamination • Soil porosity[c] • Effective depth of soil cover • Mole fractions of contaminants in waste • Absolute ambient temperature[e] • Absolute ambient pressure[e,h] • Soil bulk density[c,i] • Concentration of contaminants in soil[b] • Volume of contaminated region[b]
			With internal gas generation	• Vapor concentration of contaminants in soil pore spaces[f] • Area of contamination
		Release to ground water		- See Chapter 3.6 of Manual
	Lagoon	Volatilization		• Liquid-phase concentrations of contaminants • Area of contamination • Absolute ambient temperature[e] • Volume of contaminated region[b]
		Migration into ground water		- See Chapter 3.6 of Manual
Contaminant fate	Contaminated surface soil, landfill, lagoon	Atmospheric fate		• Distance from site to selected exposure point • Mean wind speed[e] • Relative annual frequency of wind flow towards point x[e] • Relative annual frequency of stability class for wind flow towards point x[e] • Stability classes (A = unstable, F = stable); according to Pasquill classification system[e] • Vegetative cover factor[d]

(Continued)

Table B-1. (Continued)

Type of Analysis	Type of Site	Area of Concern	Area Subclass	Parameter
		Surface water fate		• Combined effluent and stream flow data • Intermedia substance transfer rate[f] • Width of water body[j] • Stream velocity[j] • Stream depth[j] • Slope of stream channel[j]
		Ground water fate	Saturated zone	• Soil hydraulic conductivity[k] • Hydraulic gradient[l] • Effective soil porosity[k]
			Unsaturated zone	• Average percolation or recharge rate[m] • Volumetric water content of soil in unsaturated zone[f] • Hydraulic loading from manmade sources[f,n] • Precipitation rate[n,o] • Evapotranspiration rate[f,n] • Runoff rate[f,n] • Average depth of contaminated area[n] • Evaporation rate[o]
Exposed populations	All	General		• Location of population • Number of persons • Age/sex distribution
		Contaminated surface water		• Recreation patterns (fishing, hunting, swimming) • Commercial fisheries present • Drinking water intake locations and populations served
		Contaminated ground water		• Drinking water intake locations and populations served

[a] Some values can be obtained from existing literature.
[b] For calculation of long-term release (≥ 70 years).
[c] Can be obtained from Soil Conservation Service (SCS) "Soils 5 File" data base.
[d] Estimated indirectly from site survey information.
[e] Can be estimated based on existing meteorological station data.
[f] Can be calculated.
[g] Can be obtained from SCS office or from existing literature.
[h] Necessary only if diffusion coefficients for toxic components are not available from existing literature.
[i] Can be measured as an alternative to measuring soil porosity.
[j] Can be obtained from USGS data.
[k] Can be calculated or estimated from Table in Manual.
[l] Can be obtained from USGS or local university geology/hydrogeology departments.
[m] Can be calculated via equation in manual, or can be obtained from USGS, USDA, NOAA, or U.S. Forest Service.
[n] Needed to calculate average percolation/recharge rate when not measured at site.
[o] Available from local or National Weather Service.

Table B-2. Index to Variable Terms

Term Used	Definition	Units	Equation(s) in which term is used	Source
E	Potential annual wind erosion soil loss	(mass/area/time)	2-1	calculated
I'	Soil erodibility index	(dimensionless)	2-1	site data and literature
K'	Soil ridge roughness factor	(dimensionless)	2-1	site data and literature
C'	Climatic factor	(dimensionless)	2-1	literature
L'	Field length along the prevailing wind direction	(feet)	2-1	site data and literature
V	Vegetative cover factor	(dimensionless)	2-1	site data
E_{VT}	Emission factor for vehicular traffic	(kg/vehicle kilometer traveled; lb/vehicle mile traveled)	2-2	calculated
k	Particle size multiplier	(dimensionless)	2-2	see text
s	Silt content	(%)	2-2	site data, SCS Soils 5 File
S_p	Mean vehicle speed	(kph; mph)	2-2	site data
W	Mean vehicle weight	(Mg; tons)	2-2	site data
w	Mean number of wheels	(dimensionless)	2-2	site data
D_p	Number of days with at least 0.254 mm (0.01 in) of precipitation per year	(dimensionless)	2-2	Figure 2-3
E_i	Emission rate of toxic component i	(g/sec)	2-3; 2-8; 2-9; 2-11; 2-15	calculated
D_i	Diffusion coefficient of component i	(cm^2/sec)	2-3; 2-4; 2-5; 2-12	calculated
A	Contaminated area	(cm^2; areas; ha) (100 in^2)	2-3; 2-8; 2-9; 2-11; 2-15; 2-19; 2-21; 2-24; 2-25; 2-26; 2-30; 2-32; 2-33; 2-37	site data
C_{si}	Saturation vapor concentration of component i	(g/cm^3)	2-3; 2-7	calculated
P_t	Soil porosity	(dimensionless)	2-3; 2-6; 2-12; 3-17; 3-34; 3-35	site data; SCS Soils 5 File
d_{sc}	Effective depth of soil cover	(cm)	2-3	site data
M_i	Mole fraction of toxic component i in the waste	(g/g)	2-3	site data
T	Temperature	(K, C)	2-4; 2-7; 2-10; 2-13; 2-16; 2-17	site data
MW_i	Molecular weight of contaminant i	(g/mole)	2-4; 2-5; 2-7; 2-10; 2-17	literature
MW_a	Molecular weight of air	(g/mole)	2-4	see text
ΣV_1, ΣV_2	Molecular diffusion volumes of toxic contaminant (V_1) and air (V_2)		2-4	literature and calculated
P_a	Absolute pressure	atm	2-4	site data
D'	Known diffusion coefficient of a compound with molecular weight and molecular diffusion volume close to that of the unknown (D_i)		2-5	see text
MW'	Molecular weight of the selected compound corresponding to D'	(g/mole)	2-5	literature
β	Soil bulk density	(g/cm^3)	2-6; 2-25; 2-26; 2-27; 3-17	site data; SCS Soils 5 File

(Continued)

Table B-2. (Continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
ρ	Particle density	(g/cm^3)	2-6	see text
p	Vapor pressure of the chemical	(mm Hg)	2-7; 2-37	literature or estimated (see text)
R	Gas constant	(62.3 mm Hg-liter/ k-mol; 8.2 x 10^{-5} atm-m^3/-mol-k)	2-7; 2-13; 2-16	see text
C_i^*	Vapor concentration of compound i	(g/cm^3)	2-8; 2-9	site data
V_y	Mean landfill gas velocity in the soil pore spaces	(cm/sec)	2-8	see text
k_{iG}	Gas-phase mass transfer coefficient of chemical i	(cm/s)	2-9; 2-10; 2-16	calculated
MW_{H_2O}	Molecular weight of water	(g/mole)	2-10	see text
k_iG,H_2O	Gas phase mass transfer coefficient for water vapor at 25°C		2-10	calculated
C_s	The liquid-phase concentration of component i	(g/cm^3)	2-11; 2-14; 2-15; 2-19; 2-34	site data
C_B	Bulk contaminant concentration in soil	(g/cm^3)	2-11; 2-14; 2-19	site data
t	Time measured from sampling time	(seconds)	2-11	site data
d	Depth of dry zone at sampling time	(cm)	2-11; 2-14; 2-19	site data
D	Related to the amount of contaminant i that goes from liquid to gas phase, and then from gas phase to diffusion in air	(cm^2/sec)	2-11; 2-12; 2-14; 2-19	calculated
H_i'	Henry's Law constant in concentration form	(dimensionless)	2-12; 2-13	calculated
H_i	Henry's Law constant	(atm-m^3/mol)	2-13; 2-16	literature
h	Depth from soil surface to the bottom of the contaminated region	(cm)	2-14	site data
t_d	The time at which all contaminant has volatized from the soil	(sec)	2-14	calculated
K_i	Overall mass transfer coefficient	(cm/sec)	2-15; 2-16	calculated
k_{iL}	Liquid phase mass transfer coefficient	(cm/sec)	2-16; 2-17	calculated
MW_{O_2}	Molecular weight of oxygen	(g/mole)	2-17	see text
k_{L,O_2}	Liquid phase mass transfer coefficient for oxygen at 25°C		2-17	literature
E_{Ai}	Average release of contaminant i	(mass/time)	2-18; 2-19; 2-29	calculated
V_c	Volume of contaminated region	(cm^3)	2-18; 3-34; 3-35	site data
C_i	Concentration of contaminant i in soil	(g/cm^3, kg/ha, lb/acre)	2-18; 2-25; 2-26; A-3	site data
E	Total release rate of contaminant i obtained by summing all above-listed releases of the contaminant at the site	(g/sec)	2-18	calculated
$Y(S)_E$	Sediment yield in tons per event	(metric tons)	2-20; 2-27	calculated
a	Conversion constant		2-20; 2-21; 2-23; 2-24	see text
V_r	Volume of runoff	(acre-feet, m^3)	2-20; 2-21	calculated
q_p	Peak flow rate	(ft^3/sec, m^3/sec)	2-20; 2-24	calculated
K	The soil-erodibility factor. Obtained from the local Soil Conservation Service Office	(commonly expressed in tons per acre per R unit)	2-20; 2-30	site data, literature
L	The slope-length factor	(dimensionless)	2-20; 2-30	see Figures 2-4 through 2-6
S	The slope-steepness factor	(dimensionless)	2-20; 2-30	see Figures 2-4 through 2-6
C	The cover factor	(dimensionless)	2-20; 2-30	see text and Table 2-4

(Continued)

Table B-2. (Continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
P	The erosion control practice factor	(dimensionless)	2-20; 2-30	see text
Q_r	Depth of runoff	(in, cm)	2-21; 2-22; 2-24; 2-28	calculated
R_t	The total storm rainfall	(in, cm)	2-22; 2-24; 2-28	National Climatological Data Center, Asheville, NC; USDC (1961)
S_w	Water retention factor	(in, cm)	2-22; 2-23; 2-24	calculated
CN	The SCS Runoff Curve Number	(dimensionless)	2-23	Table 2-6
T_r	Storm duration	(hour)	2-24	National Climatological Data Center, Asheville, NC; USDC (1961)
S_s	Sorbed substance quantity	(kg, lb)	2-25; 2-27	calculated
D_s	Dissolved substance quantity	(kg, lb)	2-26; 2-28	calculated
Θ_c	Available water capacity of the top cm of soil	(dimensionless)	2-25; 2-26	calculated (see text)
K_d	Sorption partition coefficient	(cm^3/g)	2-25; 2-26; 3-17; 3-19	literature
PX_i	Sorbed substance loss per event	(kg, lb)	2-27	calculated
PQ_i	Dissolved substance loss per event	(kg, lb)	2-28	calculated
B	Dissolved *or* sorbed loss per storm event	(kg, lb)	2-29	calculated (see text)
N	Number of "average" storm events in 70 years	(dimensionless)	2-29	National Climatological Data Center, Asheville, NC; USDC (1961) (see text)
$Y(S)_A$	Annual soil loss in runoff	(tons)	2-30	calculated
R_r	Rainfall and runoff factor	(dimensionless)	2-30	
S_d	Sediment delivery ratio	(dimensionless)	2-30; 2-31	calculated
D_d	Overland distance between site and receiving waterbody	(Ft)	2-31	site data
L_c	Contaminant Loading rate	(mass/time)	2-32; 2-34; 2-37	calculated
C_o	Solubility of solid chemical	(mass/volume)	2-32	literature
Q_l	Volume loading rate	(volume/time)	2-33; 2-34	calculated
b	Soil specific exponential function	(dimensionless)	2-33; 3-13	Table 3-11
K_s	Soil hydraulic conductivity	(length/time)	2-33; 3-9;3-13	site data, Table 3-8; 3-9
i	Hydraulic gradient	(dimensionless)	2-33; 3-9	site data
K_c	Hydraulic conductivity of liquid contaminant in site soil	(length/time)	2-35; 3-16	calculated
K_w	Hydraulic conductivity of water in site soil (same as K_s)	(length/time)	2-35; 3-16	site data
D_c	Density of liquid contaminant	(mass/volume)	2-35	literature
D_w	Density of water	(mass/volume)	2-35	literature
u_c	Dynamic viscosity of liquid contaminant	[mass/(length × time)]	2-35	literature
u_w	Dynamic viscosity of water	[mass/(length × time)]	2-35	literature

(Continued)

Table B-2. (Continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
P_s	Permeation rate	[g-mil/ (100 in^2 × day × cmHg)]	2-36; 2-37	calculated
Ap	Permeation constant for polymer	[g-mil/ (100 in^2 × day × cmHg)]	2-36	Table 2-7
S_H	2nd permeation constant for polymer	(cc/cal)	2-36	Table 2-7
ϕ	Permachor value for polymer-permanent pair	(cal/cc)	2-36	Table 2-7; 2-9; 2-10
d_l	Thickness of liner	(mils)	2-37	site data
x	Distance from site to selected exposure point	(length)	3-1; 3-2; 3-3; 3-7; 3-8	site data
$\bar{C}(X)$	Atmospheric concentration of substance at distance X from the site	(mass/volume)	3-1; 3-3, A-1	calculated
Q	Release rate of substance from site to atmosphere	(mass/time)	3-1	calculated
σ_y	Atmospheric dispersion coefficient in the lateral (crosswind) direction	(length)	3-1; 3-3	Figure 3-5
σ_z	Atmospheric dispersion coefficient in the vertical direction	(length)	3-1	Figure 3-6
μ	Mean wind speed	(length/time)	3-1	site data
π	The value pi = 3.1416	(dimensionless)	3-1	------
$\bar{C}(X)$	Average atmospheric concentration of substance at point X over long term	(mass/volume)	3-2; A-1	calculated
W(X)	Relative annual frequency of wind flow	(dimensionless)	3-2	site data
$C_A(X)$	Atmospheric concentration at point X during stability Class A	(mass/volume)	3-2	calculated
f_A	Relative annual frequency of stability Class A for wind flow towards point X	(dimensionless)	3-2	site data
A,B,C, D,E,F	Stability classes (A = unstable, F = stable) according to Pasquill classification system	(dimensionless)	3-1; 3-2	site data
C(CL)	Predetermined critical atmospheric concentration level	(mass/volume)	3-3	air quality criteria
$Y_{(X)}$	Perpendicular distance from point X on plume centerline to the C(CL) isopleth boundary	(length)	3-3	calculated
C	Concentration of substance in stream water	(mass/volume)	3-4; 3-5; A-2	calculated
C_e	Concentration of substance in effluent	(mass/volume)	3-4	contaminant release analysis
Q_e	Effluent flow rate	(volume/time)	3-4	contaminant release analysis
Q_t	Combined effluent and stream flow rate	(volume/time)	3-4; 3-5	site data
T_r	Intermedia substance transfer rate	(mass/time)	3-5	site data, calculated
MZ	Length of mixing zone downstream of effluent release to stream	(length)	3-6	calculated
W	Width of water body	(length)	3-6	site data
u	Stream velocity	(length/time)	3-6; 3-7; 3-8	site data
d_n	Stream depth	(length units)	3-6	site data

(Continued)

Table B-2. (Continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
s_l	Slope of stream bed	(dimensionless)	3-6	site data
g	Gravitational acceleration constant	(32 ft/sec^2)	3-6	------
W(X)	Water concentration of substance at downstream distance X	(mass/volume)	3-7	calculated
W(CL)	Predetermined critical water concentration level	(mass/volume)	3-8	water quality criteria
W(O)	Water concentration of substance immediately below point of introduction to stream	(mass/volume)	3-7; 3-8	calculated
K	Overall aquatic decay coefficient	(time^{-1})	3-7; 3-8	literature, estimated
e	Exponential function	------	2-36; 3-7	------
V_{pw}	Interstitial pore-water velocity or ground-water velocity	(length/time)	3-10; 3-12; 3-18	calculated
q	Average percolation or recharge rate	(depth/time)	2-32; 3-12; 3-13; 3-14	site data, calculated
v	Darcy velocity	(length/time)	3-9; 3-10; 3-26; 3-27; 3-29; 3-30	calculated
P_e	Soil Effective Porosity	(dimensionless)	3-10; 3-11; 3-28; 3-31	site data
Θ_s	Saturated Water Content soil (equal to P_t)	(dimensionless)	3-11; 3-13	site data, literature
$\Theta_{(-15)}$	Wilting Point Moisture Content	(dimensionless)	3-11	site data, literature
Θ	Volumetric water content of soil	(dimensionless)	3-12; 3-13	site data, calculated
HL	Hydraulic loading from manmade sources	(depth/time)	3-14	site data, calculated
Pr	Precipitation rate	(depth/time)	3-14	site data
ET	Evapotranspiration rate	(depth/time)	3-14; 3-15	site data,calculated
Q_r	Runoff rate	(depth/time)	3-14	site data,calculated
EVAP	Evaporation rate	(depth/time)	3-15	site data
C_{et}	Correction factor for converting pan evaporation rate to evapotranspiration rate for turf grass	(dimensionless)	3-15	Table 3-12
C_{veg}	Correction factor for converting turf grass evapotranspiration to that for other vegetative cover	(dimensionless)	3-15	Table 3-13, see text
R_d	Retardation factor	(dimensionless)	3-17; 3-18; 3-27; 3-30	calculated
v_d	Retarded velocity of hydrophobic	(length/time)	3-18	calculated
K_{oc}	Partition coefficient for organic carbon	(ml/g)	3-19; 3-20; 3-21; 3-22; 3-23; 3-24; 3-25	calculated
f_{oc}	Fraction of organic carbon in soil	(dimensionless)	3-19	site data, literature
K_{ow}	Octanol/water partition coefficient	(ml/g)	3-20; 3-21; 3-22; 3-23; 3-24; 3-25	literature
X_d	Nomograph factor	(dimensionless)	3-26; 3-29	calculated
T_d	Nomograph factor	(dimensionless)	3-27	calculated
Q_d	Nomograph factor	(dimensionless)	3-28; 3-31	calculated

(Continued)

Table B-2. (Continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
D_X	Longitudinal Dispersion Coefficient	(length^2/time)	3-26; 3-27; 3-28; 3-29; 3-31	calculated
D_Y	Transverse Dispersion Coefficient	(length^2/time)	3-28; 3-31	calculated
m	Aquifer thickness	(length)	(Fig. 3-8)	site data
α_x	Longitudinal dispersivity	(length)	(Fig. 3-8)	literature
α_y	Transverse dispersivity	(length)	(Fig. 3-8)	literature
γ	Coefficient for decay	(dimensionless)	(Fig. 3-8)	literature
λ	Decay constant	(1/time)	(Fig. 3-8)	calculated
$T_{1/2}$	Half-life	(time)	(Fig. 3-8)	calculated
V_l	Volume of liquid chemical released	(length^3)	3-32	site data
C_l	Average concentration of chemical contaminant in released liquid	(mass/length^3)	3-32	site data
V_{gw}	Volume of contaminated ground water	(length^3)	3-32; 3-33; 3-34; 3-35	site data
C_{gw}	Average concentration of contaminant in ground water	(mass/length^3)	3-32; 3-33	site data
M_c	Mass of solid waste	(mg)	3-33	site data
C_c	Concentration Expressed as Mass Fraction	(dimensionless)	3-33	site data
IEX	Inhalation exposure	(mg/kg/day)	A-1	calculated
t_e	Duration of exposure event	(hours/event)	A-1; A-2	estimated
I	Average inhalation rate	(m^3/hr)	A-1	Table A-3
Bw	Average adult body weight	(70 kg)	A-1; A-2; A-3	Eq A-1
F	Frequency of exposure event	(number/lifetime)	A-1; A-2; A-3	estimated
DEX	Dermal exposure	(mg/kg/day)	A-2; A-3	calculated
AV	Skin surface area available	(cm^2)	A-2; A-3	estimated
PC	Dermal permeability constant for subject contaminant	(cm/hr)	A-2	Table A-4
DA	Dust adherence	(mg/cm^2)	A-3	See text
C	Contaminant concentration			

Appendix C
Data Management Forms

This appendix presents master copies of data management forms designed for use when applying the various analyses described in this manual. The forms are intended to provide easy, consistent organization of the results of each analysis component in the human exposure assessment process (qualitative analysis, quantitative contaminant release analysis, etc.) for ready use in subsequent analytical components. In addition, these forms will also organize exposure assessment output in a form most useful for conducting a risk assessment (executed following and based on the results of the exposure assessment) as well as the development of a site Endangerment Assessment for enforcement purposes.

These forms are included as master copies, that should be photocopied for use in a given site investigation. In many cases, a number of copies of certain forms will be required to tabulate all results of the exposure assessments. For example, Form No. 7: Exposure Integration requires that the exposed population segment be logged into the upper left corner of the form, and exposure information for that population segment be entered into the remaining columns for each chemical to which the population is exposed. If four distinct exposed population segments are affected at the site, four copies of the form will be required.

Form 1: Qualitative Exposure Analysis

Site Name: _____
Date: _____
Analyst: _____

Chemical	On-site Release Source	Release Likelihood/Magnitude*	Release Mechanism	Receiving Medium	Potentially Exposed Population Segment	Exposure Mechanism
1.						
2.						
3.						
4.						
5.						

Form 1. Qualitative Exposure Analysis (Continued)

Site Name: _____
Date: _____
Analyst: _____

Chemical	On-site Release Source	Release Likelihood/Magnitude*	Release Mechanism	Receiving Medium	Potentially Exposed Population Segment	Exposure Mechanism
6.						
7.						
8.						
9.						
10.						

*Code each source as to: (1) Likelihood of release and (2) Potential magnitude of release. Use H, M, L (high, medium, low) designation and provide a letter code for likelihood and magnitude, each separated by a "/".

Form 2. Quantitative Contaminant Release Data

Site Name: _____
Date: _____
Analyst: _____

Chemical	On-site Release Source	Receiving Medium	Short-term Release Rate (units)	Frequency of Short-term Release Rate (units)	Long-term Release Rate (units)
1.					
2.					
3.					
4.					
5.					
6.					
7.					
8.					
9.					
10.					

Form 3. Quantitative Environmental Fate Data

Site Name: _____
Date: _____
Analyst: _____

Chemical	Affected Medium	Short-term Environmental Concentration (units)	Long-term Environmental Concentration (units)
1.			
2.			
3.			
4.			
5.			
6.			
7.			
8.			
9.			
10.			

Form 4: Quantitative Exposed Populations Data

Site Name: _____
Date: _____
Analyst: _____

Chemical	Affected Medium	Exposure Mechanism	Population Segment (* denotes sensitive population)	Number of Persons Potentially Exposed
1.				
2.				
3.				
4.				
5.				

Form 4: Quantitative Exposed Populations Data (Continued)

Site Name: _____
Date: _____
Analyst: _____

Chemical	Affected Medium	Exposure Mechanism	Population Segment (* denotes sensitive population)	Number of Persons Potentially Exposed
6.				
7.				
8.				
9.				
10.				

Form 5: Short-terrm Exposure Calculation

Site Name: _____
Date: _____
Analyst: _____

1	2	3	4	5	6	7	8
Chemical	Exposure Mechanism	Short-term Exposure per Event (units)	Events per Time Period	Body Mass (kg)	Time Period (days)	Short-term Daily Exposure (mg/kg/day) [3 × 4E5 × 6]	Exposed Population Segment (number of persons)
1.							
2.							
3.							
4.							
5.							

Form 5: Short-terrm Exposure Calculation (Continued)

Site Name: _____
Date: _____
Analyst: _____

1	2	3	4	5	6	7	8
Chemical	Exposure Mechanism	Short-term Exposure per Event (units)	Events per Time Period	Body Mass (kg)	Time Period (days)	Short-term Daily Exposure (mg/kg/day) [3 × 4E5 × 6]	Exposed Population Segment (number of persons)
6.							
7.							
8.							
9.							
10.							

Form 6: Long-terrm Exposure Calculation

Site Name: _____

Date: _____

Analyst: _____

1	2	3	4	5	6	7	8
Chemical	Exposure Mechanism	Long-term Exposure per Event (units)	Events per Time Period	Body Mass (kg)	Time Period (2.56×10^4 days)	Long-term Daily Exposure (mg/kg/day) [3 × 4E5 × 6]	Exposed Population Segment (number of persons)
1.							
2.							
3.							
4.							
5.							

Form 6: Long-term Exposure Calculation (Continued)

Site Name: _____
Date: _____
Analyst: _____

1	2	3	4	5	6	7	8
Chemical	Exposure Mechanism	Long-term Exposure per Event (units)	Events per Time Period	Body Mass (kg)	Time Period (2.56×10^4 days)	Long-term Daily Exposure (mg/kg/day) [3 × 4E5 × 6]	Exposed Population Segment (number of persons)
6.							
7.							
8.							
9.							
10.							

Form 7: Exposure Integration

Site Name: _____
Date: _____
Analyst: _____

Population Segment	Chemical	Exposure Mechanism	Exposure: Short-term	Exposure: Long-term	Number exposed
	1. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	2. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	3. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	4. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	5. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____

Form 7: Exposure Integration (Continued)

Site Name: _____
Date: _____
Analyst: _____

Population Segment	Chemical	Exposure Mechanism	Exposure: Short-term	Exposure: Long-term	Number exposed
	6. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	7. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	8. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	9. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	10. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____

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