OSWER Directive 9285.5-1

DRAFT

SUPERFUND EXPOSURE ASSESSMENT MANUAL

Prepared for:
Office of Emergency and Remedial Response
Office of Solid Waste and Emergency Response
U.S. Environmental Protection Agency
Washington, D.C. 20460

January 14, 1986

U.S. Environmental Protection Agency
Region V, LR
230 South Dearborn Street
Chicago, Illinois 60604

U.S. Environmental Protection Agency

OSWER Directive 9285.5-1

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Superfund Exposure Assessment Manual

EPA Contract Nos.: 68-01-6271, Task No.: 59
68-03-3149, Work Assignment No. 23-2
68-01-7090, Work Assignment No. A-02

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January 14, 1986

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1.0 INTRODUCTION

1.1 Background

The Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA) was enacted to provide the Federal Government with the authority to respond to releases or substantial threats of releases of hazardous substances, pollutants, or contaminants into the environment. Pursuant to the mandates of CERCLA, procedures for the funding and execution of such responses have been developed.

In response to Section 105 of the Act, the U.S. Environmental Protection Agency was charged with the responsibility for reviewing and revising the National Oil and Hazardous Substances Contingency Plan (NCP). Among the provisions that Section 105 of the Act directed to be incorporated into the NCP during this revision effort were: (1) procedures for the identification and investigation of facilities that are releasing or may potentially release hazardous substances, pollutants, or contaminants to the environment; (2) methods for evaluating such existing or potential releases if they pose substantial danger to human health or the environment; and (3) methods for evaluating and selecting cost-effective control measures. In meeting this responsibility, EPA published the revised NCP as a final rule on November 20, 1985.

As set forth in the revised NCP (see 40 CFR Part 300), uncontrolled hazardous waste sites are to be reviewed and ranked according to their potential for release of hazardous substances. This ranking is conducted according to procedures provided in the Hazard Ranking System (HRS). Those sites that receive high HRS scores are then listed on the National Priorities List (NPL) as designated Superfund sites.* For sites listed on the NPL, a Remedial Investigation (RI) and a Feasibility Study (FS) are major components in the remedial response process. The U.S. Environmental Protection Agency has developed guidance for Remedial Investigations (USEPA 1985a) and Feasibility Studies (USEPA 1985b). A goal of the Remedial Investigation is the acquisition of field data needed to determine the extent of existing contamination at the site (in the absence of any control measures). In the Feasibility Study, these data are used to evaluate site-related exposure. The Feasibility Study also evaluates the public health impacts from exposure attributable to

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*A cut-off score has been established by EPA to differentiate those sites that score "high," and therefore require listing on the NPL, from those sites that rank "low" in this relative ranking procedure.

the uncontrolled site, and identifies and evaluates the overall effectiveness of potential remedial alternatives. The ultimate goal of the Feasibility Study is to select a cost-effective remedial alternative that provides adequate public health and environmental protection.

The public health evaluation component of the Feasibility Study defines the type and extent of hazards to public health presented by a site in the absence of remedial action. It is based in large part on an exposure assessment that evaluates: the type and extent of contaminant release from a site to environmental media; the environmental transport and transformation of contaminants following release; and the magnitude of contact with human populations. The results of the exposure assessment may aid the public health evaluation in one of two ways. Measured or estimated environmental contaminant concentrations can be compared with public health standards or criteria that identify acceptable concentrations of contaminants in specific environmental media to directly assess the potential public health impact. Alternatively, in the absence of such standards/criteria, the public health evaluation process evaluates exposure estimates in light of relevant toxicological data to determine the magnitude of the health hazard posed by the uncontrolled site.

In addition, the exposure/public health assessment is a major component of a site Endangerment Assessment (refer to USEPA 1985c for a detailed discussion of the content and application of Endangerment Assessments). The Endangerment Assessment provides the documentation of environmental and human population risk that is required before EPA can initiate an enforcement action pursuant to Section 106 of CERCLA.

This Superfund Exposure Assessment Manual is designed to complement the Superfund Public Health Evaluation Manual (USEPA 1985d), which details the information requirements and analytical procedures necessary to conduct a public health evaluation during a Feasibility Study. It also provides an analytical approach and methods useful in addressing other analyses conducted during the RI/FS. For example, many of the analytical procedures provided in this manual for the determination of contaminant release and mobility in the environment are equally well suited for the analysis of natural resource damages as required by Section 301(c) of CERCLA. Similarly, many of these procedures may also aid in the identification of potentially useful remediation technologies.

In conducting a Superfund evaluation of exposure and public health impact, the analyst initially applies the indicator chemical selection

process* as outlined in the Superfund Public Health Evaluation Manual. Once those chemicals upon which site analyses will focus have been selected, the framework for exposure assessment provided in this manual is applied. When exposure has been evaluated, the analyst returns to the Superfund Public Health Evaluation Manual for guidance in determining the degree of public health impact for each receptor population. This process is illustrated in Figure 1-1.

The procedures provided in the Superfund Public Health Evaluation and Superfund Exposure Assessment Manuals provide direct input to the evaluation of threats posed by the uncontrolled site (no-action alternative), and the development and evaluation of alternative remedial actions. Procedures and approaches for developing and evaluating these alternatives will be presented in several guidances currently under development, including guidance documents for soils and ground water remedial actions and criteria for selecting alternative technologies. Those guidances will refer the reader to the Superfund Exposure Assessment Manual for specific analytical procedures.

Many methods exist which could conceivably be applied to component portions of the analytical process outlined in following chapters; however, all possible approaches could not be addressed here. In developing this manual the authors have attempted to compile those analytical methods most appropriate for assessing human exposure to chemicals migrating from uncontrolled hazardous waste facilities. It should be noted, however, that during the review process certain potentially pertinent methods in addition to those currently addressed have been identified for consideration and possible future incorporation into this manual. Examples are the Vertical and Horizontal Spread (VHS) model for screening groundwater contamination potential, and the EP-Toxicity procedure for evaluating the leachate generation potential of certain waste constituents. Following evaluation of these procedures, their utility in conducting Superfund exposure assessments will be identified and detailed in the next revision of this manual.

EPA is developing other more detailed information to support the effective and consistent application of the RI/FS process. For example, Health Effects Assessments for contaminants likely to be found at uncontrolled hazardous waste facilities are being compiled. These provide information on the physical and chemical properties and

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*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.

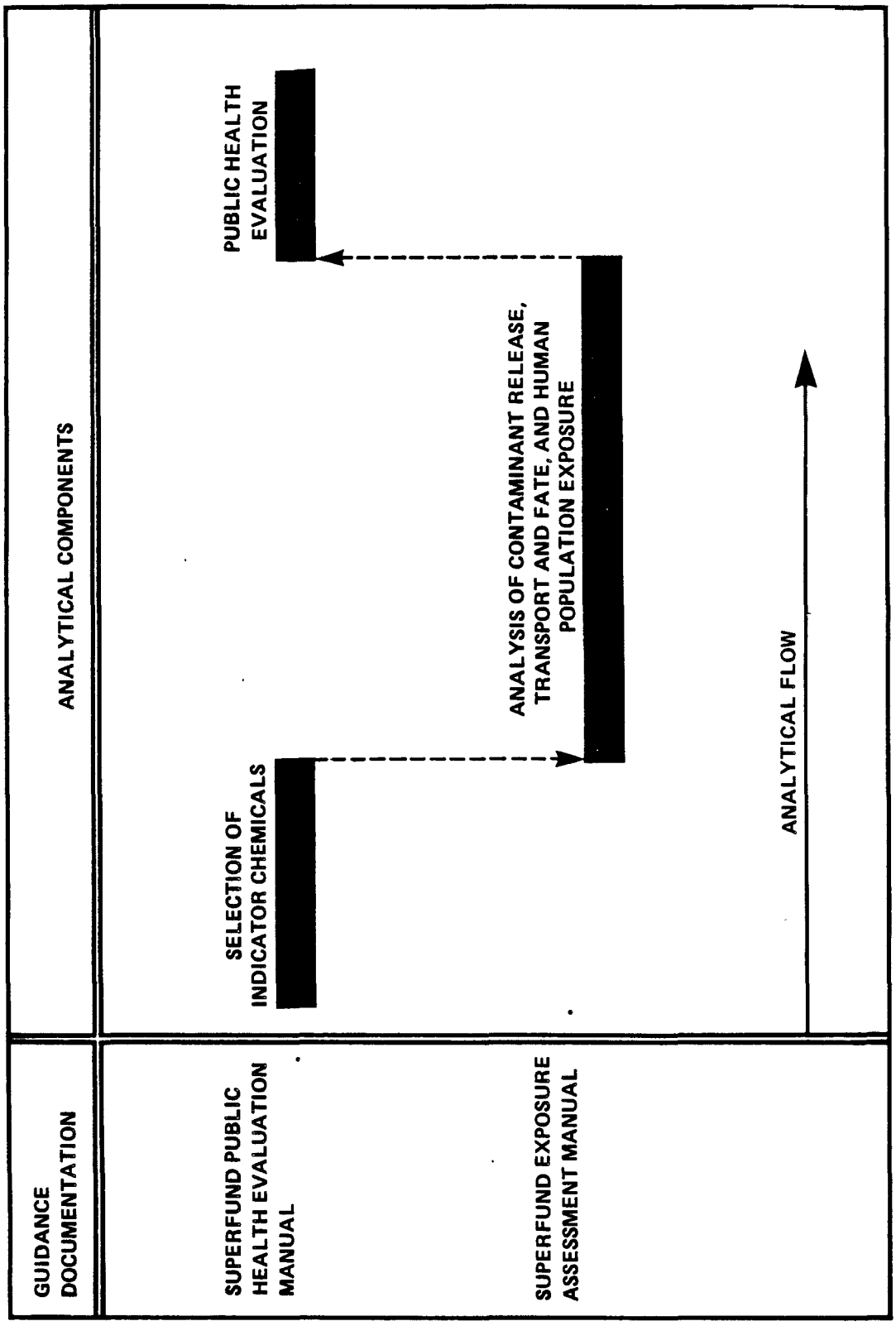

FIGURE 1-1. RELATIONSHIP BETWEEN PUBLIC HEALTH EVALUATION AND EXPOSURE ASSESSMENT GUIDANCE FOR SUPERFUND SITES

toxicological characteristics of such substances. Copies of the Health Effects Assessments are available through the National Technical Information Service. Field sampling Data Quality Objectives (DQOs) are being developed in two parts. The first part (DQO 1) will establish a phased sampling strategy designed to guide the efficient acquisition of field data for site-specific exposure and public health assessments. The second part (DQO 2) will provide sampling plan guidance addressing the location of sampling points. Field Operating Procedures for obtaining and handling samples are also being developed. Similarly, a Soil Contamination Evaluation Methodology (SOCEM) is being developed that will provide the user with a simplified procedure for determining the risk that contaminated soils pose to ground water, and for evaluating the degree of reduction in such risk attainable through implementation of various remedial alternatives. Finally, guidance for evaluating and selecting ground-water remedial actions is under development.

1.2 Purpose and Scope

This manual presents an integrated methodology designed to guide the three major component analyses required to assess human population exposure to contaminants released from uncontrolled hazardous waste sites: (1) analysis of toxic contaminant releases from a subject site, (2) determination of the environmental fate of such contaminants, and (3) evaluation of the nature and magnitude of human population exposure to toxic contaminants. These major analytical components are conducted in sequence to qualitatively or quantitatively track the migration of contaminants through environmental media to points of contact with human populations. In quantitative studies, medium-specific exposure estimates are initially developed for each chemical being evaluated, and the analysis culminates in the integration of all exposures to receptor populations.

This manual is designed for three specific purposes. First, the overall analytical process outlined herein provides a framework for the comprehensive assessment of human exposure associated with uncontrolled hazardous waste sites. It ensures that all pertinent contaminant releases and exposure routes are considered, and that an appropriate level of analytical detail is applied to each component of the evaluation to support the public health evaluation process.

Second, application of this framework supports the development of exposure assessments that are consistent from site to site. That is, application of the same analytical philosophy and overall procedure to each site will ensure that the results obtained are comparable among sites, and will provide a means of documenting that each site receives adequate evaluation.

Third, the procedures presented in this manual reflect state-of-the-art methods for conducting the various component analyses that make up an exposure assessment. However, it is recognized that contaminant release estimation, chemical fate and transport determination, etc., are developing sciences. Therefore, although the overall conceptual approach for conducting exposure assessments at Superfund sites will probably remain appropriate over time, alternative analytical methods may be developed for parts of the assessment. In such cases, the methods presented in this manual can serve as a benchmark against which such alternative methods can be compared.

1.3 Organization of the Manual

The following chapters of this manual detail qualitative and quantitative methods for evaluating human population exposure to chemicals migrating from Superfund sites. Chapter 2 broadly outlines the analytical framework. Subsequent chapters describe qualitative and quantitative analytical methods for use in each portion of the overall site analysis. Chapter 3 presents methods for evaluating contaminant release from the site; Chapter 4 addresses environmental fate analysis; and Chapter 5 details analysis of potentially exposed human populations. The results of these analyses are combined in Chapter 6, which addresses the calculation of medium-specific exposure estimates and integration of all exposures to each hazardous substance. The last chapter of the manual, Chapter 7 cites references used in developing this guidance. Appendix A contains an index to the variable terms used in the equations in Chapters 3 and 4. Appendix B provides a suggested format for documenting the exposure assessment, while Appendix C presents master copies of data management forms, designed to facilitate the recording and organization of the results obtained by applying the analytical procedures discussed in Chapters 3, 4, 5, and 6. These forms arrange data in a format useful for public health evaluation (conducted following and based on the results of the exposure assessment), as well as for development of an Endangerment Assessment for enforcement purposes.

2.0 STRUCTURE AND APPLICATION OF THE EXPOSURE ASSESSMENT PROCESS

2.1 Methodological Framework

The ultimate goal of human exposure assessment at Superfund sites is the determination of the type and magnitude of potential human population exposure to contaminants present at and migrating from the site. Depending on site conditions, this goal may be achieved by application of either qualitative or quantitative analysis. Many sites may require a mix of qualitative and either simplified or in-depth quantitative exposure analysis.

The general framework for conducting an integrated exposure analysis is broadly illustrated in Figure 2-1. Briefly, analysis of contaminant release involves identifying each on-site source of release of each target chemical to specific environmental media. Emissions are characterized as to types and amount of chemicals involved, and a determination is made of the level of release (mass loading) of each chemical to each affected medium. The results of the release analysis step provide the basis for evaluating the potential for contaminant transport or transformation and environmental fate. This analysis is also chemical- and medium-specific.

Environmental fate analysis produces results that describe the extent and magnitude of environmental contamination (i.e., contaminant concentrations in specific environmental media). This output, in turn, allows the user to predict human population contact with chemicals emanating from the site. Exposed populations analysis results in the identification, enumeration, and characterization of those population segments likely to be exposed.

The assessment concludes with an integrated exposure analysis. In this step, individual chemical-specific exposure estimates for each exposure route (i.e.; inhalation, ingestion of drinking water and/or food, dermal contact) are developed. Subsequently, individual route-specific exposures to each chemical are integrated by exposed population segment. That is, for each receptor population, all exposures to each hazardous substance are identified. In cases where 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 and work in the vicinity of a Superfund site may experience inhalation exposure while at work as well as while at home, and both of these exposures should be summed for exposure integration purposes. The results of the exposure integration provide critical input into the subsequent baseline public health evaluation process. During evaluation of remedial alternatives, however, the

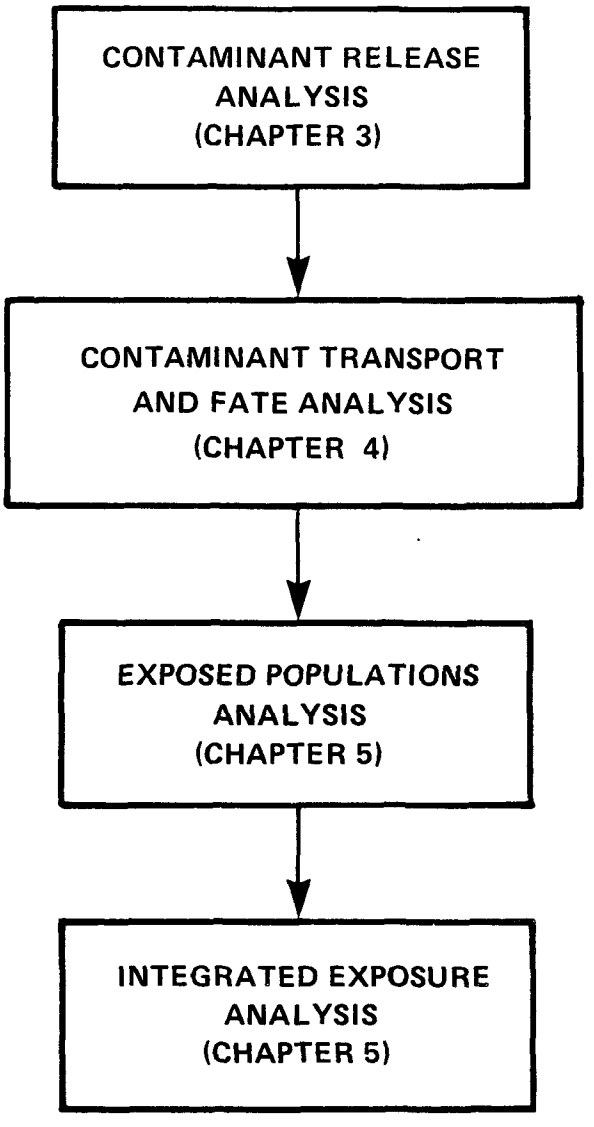

FIGURE 2-1. OVERVIEW OF THE INTEGRATED EXPOSURE ASSESSMENT PROCESS

individual route-specific exposure estimates are again important because they provide information necessary to evaluate the effectiveness of medium-specific control options.

2.2 Timeframe of Analysis

Quantitative exposure assessments generate estimates of the long-term (average) and short-term daily exposure to contaminants. For exposure evaluation purposes, these values are referred to as chronic daily intakes (CDIs) and subchronic daily intakes (SDIs), respectively. The output of each analytical component (contaminant release, environmental fate, etc.) must be expressed in the same form. That is, contaminant release analysis will generate long-term and short-term contaminant release values, and environmental fate analysis will project long-term and short-term contaminant concentrations in environmental media. 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 for public health assessment purposes (see USEPA 1985d) as those that occur over a short period (usually 10 to 90 days) during the first year following site investigation, since it is expected that release rates will decrease over time as the on-site contaminant reservoir decreases. For contaminant fate analysis, long-term and short-term values are a function of the extent of contamination, with long-term values being the average over time of environmental concentrations of each contaminant and short-term values being the highest calculated concentration in each affected medium.

2.3 Exposure and Dose

It is important to distinguish between exposure and dose. The dose of a chemical incurred by a receptor is determined by the degree to which the chemical is transferred across the body membranes it contacts. For many chemicals, absorption may be 100 percent; in such cases, dose equates with exposure. In other cases, however, less than total absorption may occur. The degree of absorption may vary, for example, depending on where the chemical contacts the body (e.g., in the gut, in the lungs, on the skin). When absorption data are lacking, as is often the case, it is common to conservatively assume total absorption and let the exposure value represent the dose incurred.

2.4 Exposure Assessment Flexibility and Complexity

Many analytical approaches and tools can be applied to the exposure assessment process. They can be expensive or inexpensive to apply and can result in low or high quality analytical results. The key to selection of specific analytical methods is to conduct analyses that are appropriate for the site and situation in question.

The user of this Manual should understand that the analytical framework and procedures presented herein are intended to be applied to Superfund site exposure assessments in a flexible manner. No two sites will be exactly alike in terms of the extent and complexity of contamination, of contaminant migration, or of potentially exposed populations. Some parts of the overall exposure assessment process will not be required to adequately assess exposure potential at some sites. Therefore, the approach and methods applied to conducting an exposure assessment should be tailored to address existing site conditions. Often some contaminant releases or exposure routes may be adequately addressed by applying only screening procedures. In other cases more complex, quantitative evaluation will be necessary. Thus, the overall exposure assessment process as applied to any given site should be viewed as a continuum, wherein analytical methods of varying detail and complexity are applied, as appropriate, to specific component portions of the site evaluation.

In the Superfund Public Health Evaluation Manual (USEPA 1985d, p. 9), five factors affecting the degree of analytical complexity for site analyses are listed:

- number and identify of chemicals present;
- availability of appropriate standards and/or toxicity data;
- number and complexity of exposure pathways (including complexity of release sources and transport media);
- necessity for precision of the results, which in turn depends on site conditions such as the extent of contaminant migration, proximity, chracteristics and size of potentially exposed populations, and enforcement considerations (additional quantification may be warranted for some enforcement sites); and
- quality and quantity of available monitoring data.

Sites where only a small number of chemicals require evaluation, where environmental standards or criteria for chemicals under study are available, where a small number of exposure pathways are present; where release and transport processes are relatively simple, or where only a limited need for detail and precision in the assessment results exists may require only simplified analysis. Conversely, sites with many contaminants for which no environmental standards or criteria are available, which exhibit multiple exposure pathways, which have complex contaminant release and transport processes in effect, or for which analytical results of high detail and precision are required will

necessitate application of more complex, quantitative analytical methods. Note, however, that most sites will fall somewhere between these two extremes.

The concept of an analytical continuum also applies to each component evaluation in the exposure assessment process. For example, initial contaminant release analysis may be predominantly qualitative to develop a preliminary screening of on-site contaminant release sources.. From this screening analysis, the existence of any complete exposure pathways is determined, targeting of key exposure routes is initiated, potentially applicable prevention or remediation technologies are identified, and the requirements for more detailed quantitative analysis of releases (if necessary) are determined. Subsequent quantitative analyses of increasing complexity can then be conducted to develop data of appropriate detail. This same approach is applied to analysis of contamination migration and fate and of population exposure.

As previously mentioned, analytical tools of varying degrees of complexity and resource-intensiveness are available for Superfund site analyses. 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 in this latter category. Generally, it will be appropriate to apply simplified analysis to all pertinent exposure routes at the initiation of quantitative evaluations so that those of greatest concern can be identified for subsequent in-depth analysis.

This progression from screening evaluation of the overall site to increasingly detailed and targeted quantitative analysis allows site evaluations to be conducted in a manner that maximizes analytical cost-effectiveness. The most resource-intensive analytical tools are applied only to those exposure routes of greatest concern; unnecessary analysis is avoided while obtaining results of maximum utility. Often, however, initial screening analysis may itself point out the need for in-depth quantitative analysis of particular pathways. For example, this may occur if high risk populations, very large amounts of contaminant, or highly toxic substances are involved. In such cases, simplified quantitative analysis components may be bypassed for specific pathways, and in-depth procedures would be directly applied. In addition, it should also be noted that in some cases the results of either screening or simplified quantitative analyses may directly point to the requirement for a specific remedial alternative, thereby negating the need to conduct additional, more resource-intensive analysis.

2.5 Exposure Assessment Output and Report Format

The results of both the exposure and the public health assessments provide critical information for those responsible for the selection and implementation of remedial options at Superfund sites. For Fund-financed Remedial Investigations/Feasibility Studies, exposure assessment results should be presented in the public health chapter of the Feasibility Study report. This section of the report will present the qualitative and quantitative results of the exposure assessment and will document development of integrated exposure estimates for each contaminant under study. However, the exposure assessment must detail more than the end result of the analyses conducted. In order to efficiently provide certain information needed for analysis of baseline conditions and remedial alternatives, as well as for project documentation purposes, it should describe the information used, analyses conducted, and results obtained, as well as the assumptions and uncertainties to be considered when interpreting the results. This information will be critical for all sites that are not clearly no-action sites, since these analyses may be revised and expanded when formulating and evaluating different remedial alternatives.

It is suggested that each exposure assessment begin with a summary of the type and magnitude of hazardous substance release, migration, and associated human population exposure. The summary should discuss the purpose of the exposure assessment (i.e., to develop exposure data necessary to support development of a public health evaluation) and describe the scope of the assessment. Subsequent sections should parallel the various analytical components that make up the exposure assessment process: contaminant release analysis, contaminant environmental fate analysis, exposed populations analysis, development of medium-specific exposure estimates, and exposure integration. Appendices to the Feasibility Study report may present information developed during the exposure assessment on the data management forms that are provided with this manual. This will facilitate extraction of relevant data for use in the subsequent public health evaluation and remedial alternatives evaluation processes.

2.6 Application of the Exposure Assessment Process

For any given site, the methods discussed herein are applied during the Feasibility Study to analyze the existing situation, i.e., the baseline condition. This analysis equates with evaluation of the "no action alternative."

The same analytical procedures used in evaluating the baseline condition may also be used during the Feasibility Study to analyze the post-remediation effectiveness of remedial alternatives. This essentially involves applying the exposure assessment process in reverse. That is, beginning at the point(s) of exposure, acceptable exposure levels (described in the Superfund Health Evaluation Manual, USEPA 1985d) can be converted into associated environmental concentrations based on pertinent intake rates (ingestion, inhalation) and dermal contact values (e.g., daily exposure ÷ liters of water ingested = concentration). For alternatives developed to mitigate contamination already migrating from the site (management of migration measures), the uncontrolled concentration minus an acceptable concentration can provide a target level of migration control (i.e., concentration reduction) that must be achieved to adequately protect human health.

For alternatives intended to control the source of contamination (source control measures), cleanup goals are designed to reduce or eliminate the release of contaminants from the site. Therefore, in order to evaluate the effectiveness of source control alternatives, an acceptable contaminant release term is required. This can be developed by using the acceptable environmental concentration value to estimate an acceptable release rate. This acceptable release rate can be subtracted from the uncontrolled release rate to yield a target release reduction for on-site remedial alternatives. Similarly, if contaminant removal is being considered, the acceptable release rate can be converted into acceptable on-site concentrations which, when subtracted from uncontrolled on-site concentrations, provide a target contaminant concentration reduction value. The Superfund Public Health Evaluation Manual and the guidance for soils and ground water remedial actions will provide detailed direction for conducting this remediation design-based analysis. Many of the analytical methods discussed herein can be used to directly calculate the required acceptable values. Specifically, the equations provided for quantitative estimation of contaminant release or transport can be adapted to allow solution for soil concentrations or release rates. In other cases, such as many computerized models, the analysis may have to be conducted in an iterative fashion. Many computerized environmental fate models can only solve for concentration in the medium being modeled. In such cases, hypothetical release rate values must be repeatedly input into the model and the associated concentration calculated until the target concentration is approximated. The hypothetical release rate input in this case would then equate with the acceptable release rate that remediation can be targeted to achieve.

An additional purpose served by this manual is the identification of site data required to conduct various component analyses that may be needed to develop estimates of contaminant release and transport. For convenience, possible data requirements are summarized in Table 2-1, and are detailed in Appendix A. The analyst should become familiar with these data needs prior to initiating analysis so that appropriate data (developed during the Remedial Investigation, estimated, or available from the literature) can be readily accessed to support the exposure assessment process. As previously mentioned, EPA is currently developing guidance for Remedial Investigation data acquisition activities. A major component of this guidance consists of Data Quality Objectives (DQOs). These will establish a phased approach to field data acquisition. That is, initial data collection will be designed to support site screening. This will typically involve acquisition of data adequate to characterize the hazardous substances present at the site, identify the mode of their disposal on-site, and roughly evaluate the amounts present. These data will support a simplified exposure pathway evaluation, such as those being developed for the Soil Contamination Evaluation Methodology, to roughly gauge the existence and magnitude of contaminant migration pathways and exposure potential, and will provide a basis for preliminary consideration of potential remedial alternatives. These rough analyses should be initiated at the early scoping stages of the RI. The SOCEM and Superfund Exposure Assessment Manual will provide simplified, non-data-intensive analytical tools that can be used at this stage. Subsequently, additional targeted sampling or monitoring will be conducted to support more precise determination of the existing exposure potential and definition of remedial technology design parameters. Thus, field data acquisition conducted in accordance with the Data Quality Objectives and the SOCEM will ensure that data are adequate to support the development of screening as well as simplified or in-depth quantitative exposure assessment.

Table 2-1. 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[c] • 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

Table 2-1. (continued)

Type of analysis	Type of site	Area of concern	Area subclass	Parameter
Contaminant release (continued)	Contaminated surface soil (continued)	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 3.4 of Manual
	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

Table 2-1. (continued)

Type of analysis	Type of site	Area of concern	Area subclass	Parameter
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 A for wind flow towards point x[e] • Stability classes (A = unstable, F = stable); according to Pasquil classification system[e] • Vegetative cover factor[d]
		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]

Table 2-1. (continued)

Type of analysis	Type of site	Area of concern	Area subclass	Parameter
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

Table 2-1. (footnotes)

[a]Some values can be obtained from existing literature.

[b]For calculation of long-term release ($\geq$ 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.

3.0 CONTAMINANT RELEASE ANALYSIS

3.1 Introduction

This chapter provides guidance for analyzing contaminant releases from uncontrolled hazardous waste facilities. The first step of the analysis is an evaluation of available site data to determine their completeness and adequacy, and to identify data gaps. An evaluation of the likelihood and extent of contaminant release from a site depends on data that define the chemical and physical properties of the contaminants present, describe the climatological regime predominant in the area, and identify the location and manner of waste placement at the site (e.g., buried in landfill, present in surface lagoon, stored above ground in leaking drums, etc.). Once the requisite site data are acquired, each potential on-site source of contaminants is identified and evaluated to determine its contribution to overall site contaminant loading.

A variety of analytical tools and techniques can be applied to the exposure assessment. To determine the type and extent of analysis required for each potential release source, an initial screening is conducted of contaminant release mechanisms in evidence at the site. This screening is a qualitative evaluation of site conditions that (1) identifies each potential contaminant release source, (2) determines the environmental media affected by such releases, and (3) broadly defines the likely magnitude of release. The following subsection provides guidance for this screening through explanatory text and accompanying decision networks. It is designed to establish a consistent basis for qualitative contaminant release screening from site to site.

This guidance provides four distinct benefits for the RI/FS analysis. First, it constitutes an organized basis for identification of existing (baseline) and potential contaminant releases. Second, contaminant release screening results in a rough determination of the relative magnitude of the various contaminant sources associated with the site. This provides a basis for planning the type and extent of subsequent quantitative analysis. Releases that appear to be relatively minor can be scheduled for simplified, "desk top" quantitative estimation, while for major releases it may be appropriate to directly apply more sophisticated in-depth procedures (i.e., monitoring or computer modeling). Similarly, release screening identifies data gaps that must be filled in order to conduct quantitative analyses. Third, the screening results provide information necessary to initially identify remedial technologies that may be appropriate for implementation at the site. Fourth, application of screening procedures assures that analyses of baseline and remediation scenarios are conducted in a comprehensive and consistent manner. Their use assures that baseline releases as well

as any additional contaminant releases associated with implementation of given remediation technologies are considered, and that analyses conducted among different sites are comparable.

3.2 Contaminant Release Screening

Depending on the manner of placement of wastes at an abandoned site, contaminant release* may occur by any or all of the mechanisms summarized in Table 3-1. In contaminant release screening, the likelihood of release from each source is considered as well as the nature of the contaminants involved and the probable magnitude of their release (relative to other on-site sources).

Figures 3-1 and 3-2 present the decision networks that constitute the methodological framework to guide contaminant release screening analysis. Figure 3-1 deals with contaminants in or under the soil, while Figure 3-2 addresses above-ground wastes. On both figures, "dead end" boxes (yes/no) indicate that further evaluation of a potential release mechanism is not necessary. Any release mechanisms that are determined in this qualitative evaluation to be in evidence at the site will require further screening evaluation to determine the likely environmental fate of the contaminants involved (see Chapter 4). In Sections 3.2.1 and 3.2.2 below, brief guidance for the qualitative evaluation of on-site sources of potential contaminant release to the evironment is provided. The paragraphs presented in each section are keyed to the accompanying decision networks, and are intended to provide additional insight into those boxes on the networks that may not be entirely self-explanatory.

3.2.1 Contaminant Release Screening: Contaminants in Soil (see Figure 3-1):

The following numbered paragraphs are provided to facilitate interpretation and application of the contaminant release decision network presented as Figure 3-1. Each paragraph refers to a particular numbered box in the figure.

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

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*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, etc. are considered to be release mechanisms. Contaminant transport is considered to equate with those processes that carry released contaminants to points distant from the site.

Table 3-1. Potential Contaminant Release[1] Mechanisms

Process	Media directly affected (media indirectly affected)	Time frame
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 3.2 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.

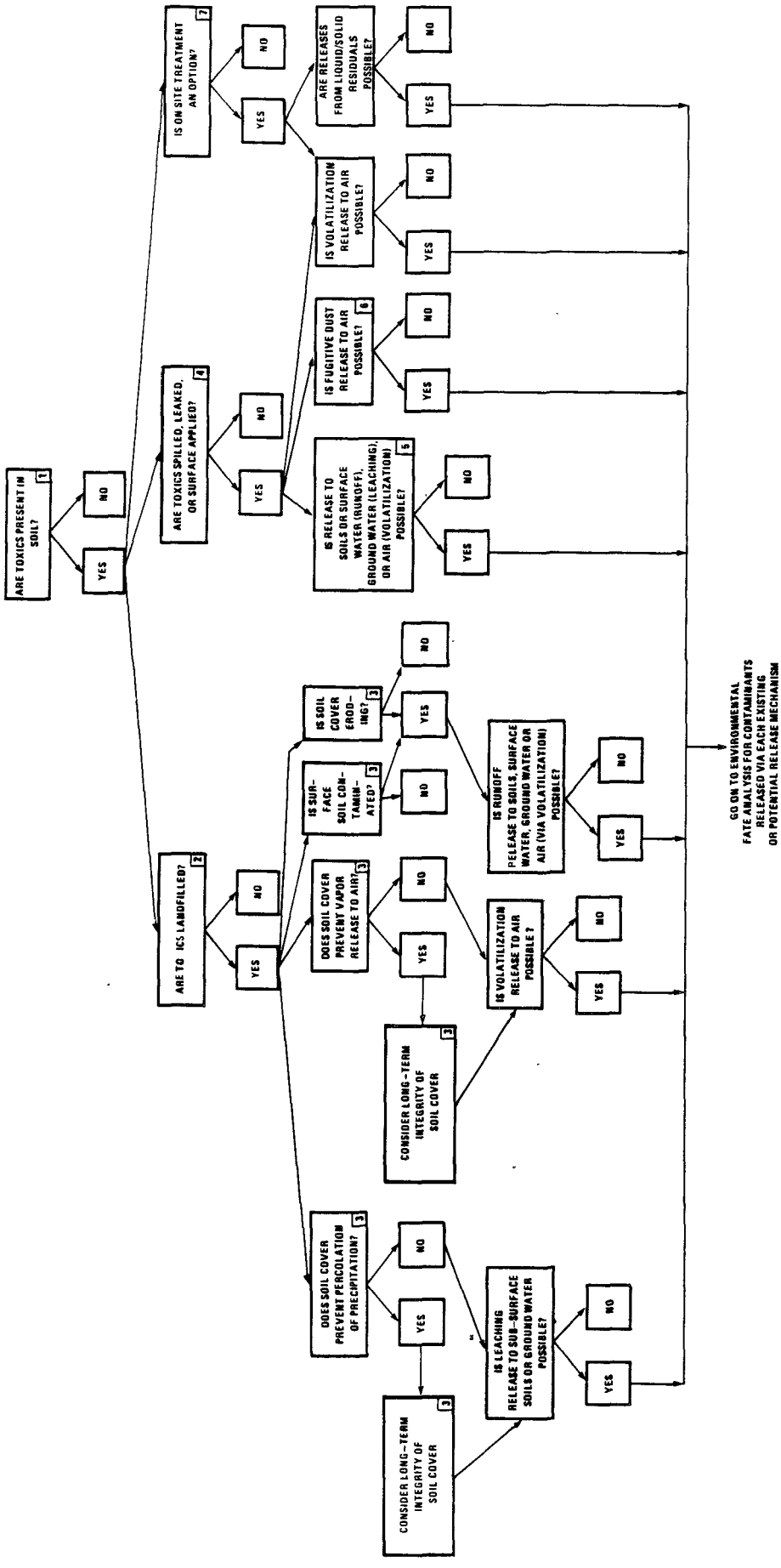

FIGURE 3-1. CONTAMINANT RELEASE DECISION NETWORK: CONTAMINANTS IN SOIL

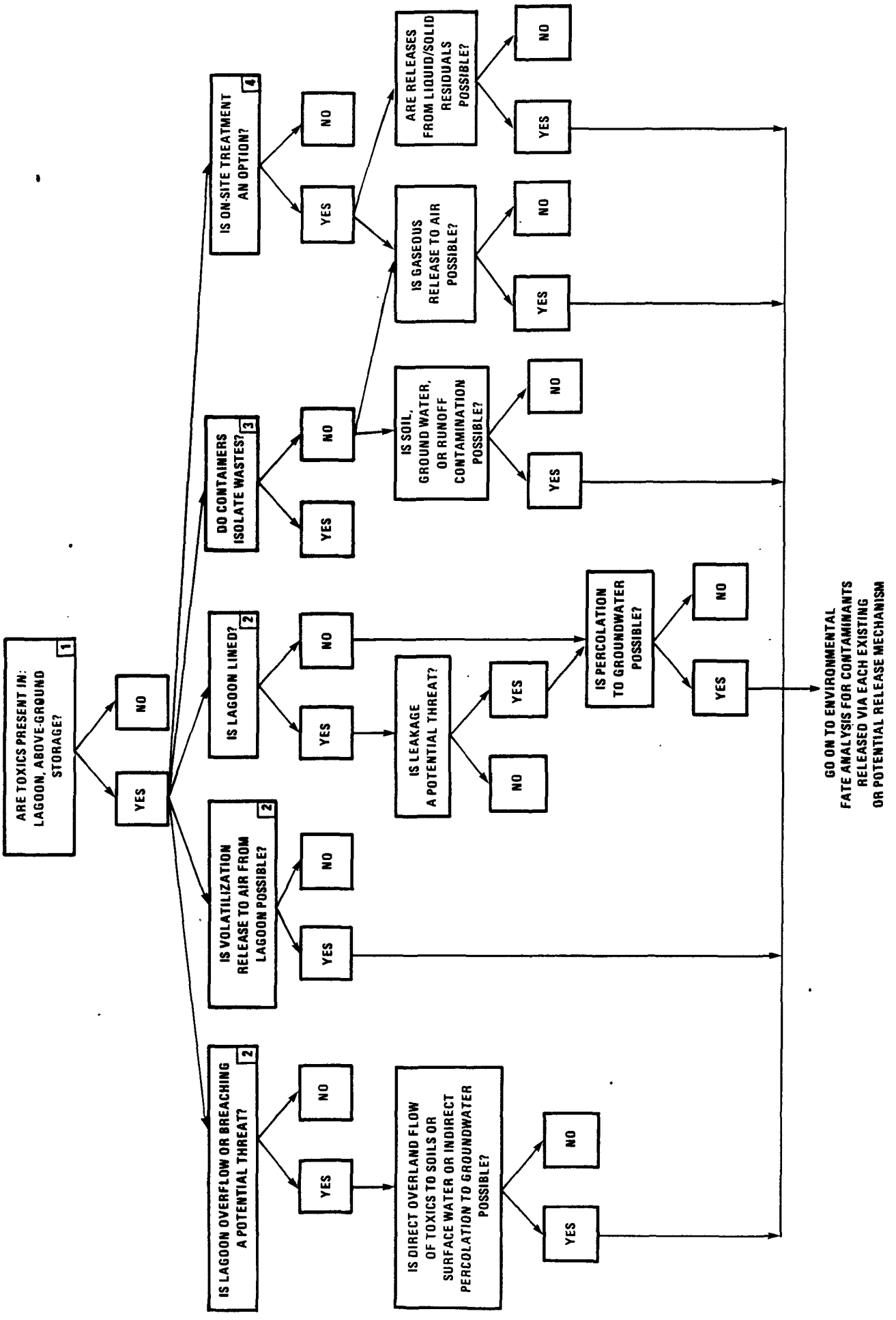

FIGURE 3-2. CONTIMINANT RELEASE DECISION NETWORK: CONTAMINANTS ABOVE GROUND

2. Landfilled wastes may become mobilized if they are not contained in impervious containers, or if containers are leaking. Release of such wastes may contaminate subsoils, ground water via percolation, or air via 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 may contaminate subsoils and ultimately reach ground water. Similarly, the soil cover may not be deep enough to preclude the migration of volatile contaminants upward into the atmosphere. It has been estimated that about 60 percent of hazardous waste is in liquid (sludge) form (USEPA 1980a). Infiltrating rainwater can increase the migration rate of liquid or semi-liquid materials by increasing the hydraulic head affecting them, as well as by leaching of toxic components. Erosion, extreme drying (and cracking), etc. can reduce the ability of a soil or clay cover to maintain isolation of wastes. Also, waste cells may themselves be covered with contaminated soil. When evaluating the potential for landfill releases, the long-term integrity of the landfill and its soil cover should be evaluated as well as its current condition. If the landfill soil cover does not assure long-term isolation of the wastes, the leachability and volatilization potential of the landfilled wastes should be evaluated.

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. Similarly, at most sites surface soils have become contaminated because of hazardous material spills or leaks during manufacture, processing, storage, or transfer operations. In such situations, the potential for release of contaminants in surface soils via four mechanisms should be evaluated. These 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/leaching to ground water.

5. Surface soils and underlying ground water may become contaminated by percolation of contaminated runoff, and surface water systems may be similarly degraded by contaminated runoff inflow. Runoff may also serve as a source of volatilization release to air, although such release directly from contaminated soils would be expected to constitute a greater threat than that from contaminated runoff. Hydrophobic wastes may contaminate surface water bodies 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 long periods of time.

6. Wind erosion may carry solid particulate wastes or soil particles with adhered hydrophobic toxic materials from the site during high wind conditions.

7. In many cases, on-site treatment of hazardous wastes may be possible. In such cases, the contaminant release potential of the treatment process(es) employed should be evaluated. Incineration of hazardous wastes can achieve high destruction and removal efficiencies, thereby releasing negligible amounts of toxics to the atmosphere under normal operatin conditions. Incineration may be appropriate for high BTU wastes that do not contain a high heavy metal content. Consideration should be given, however, to the potential for formation of toxic reaction products when the principal organic hazardous constituents are incinerated, as well as to any potential operational problems that may reduce the system's contaminant destruction efficiency.

Other treatment technologies in effect are media-shift operations. For example, air or steam stripping forces evaporation of volatile contaminants from water to air. Similarly, artificially aerated biological treatment processes may also promote release of volatiles. In many cases, treatment itself may generate residual waste streams that contain hazardous components and require further treatment or proper disposal. In any case, the direct and indirect releases (fugitive and process emissions, effluents, sludges, and solid wastes) associated with waste treatment options considered for use at Superfund sites should be evaluated for their contaminant release potential.

3.2.2 Contaminant Release Screening: Contaminants Above Ground (see Figure 3-2):

The following numbered paragraphs are provided to facilitate interpretation and application of the contaminant release decision network presented as Figure 3-2. Each paragraph refers to a particular numbered box in the figure.

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

2. Lagoons may introduce hazardous materials to the environment via a number of pathways. Breaching of the lagoon due to erosion or overflow resulting from heavy rainfall can result in outflow of liquid wastes that contaminate surface soils, ground water, and surface water bodies. Unlined lagoons may introduce toxics directly into ground water via percolation through the lagoon bottom. Also, because lagoons are uncovered, 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 is a common problem. Leaked wastes will contaminate soils in the storage area may percolate to ground water, or may contaminate surface runoff which can, in turn, further extend the area of soil contamination or enter local surface water bodies. If volatile, leaked materials will evaporate into the atmosphere.

4. As previously mentioned, various on-site treatment options may themselves result in potential hazardous substance release to the environment. Potential emissions, effluents, sludges, and solid wastes resulting from on-site treatment should be evaluated for their contaminant release potential.

3.3 Quantitative Contaminant Release Analysis

Once potential on-site contaminant release sources have been screened, those requiring further evaluation are quantitatively analyzed. This may involve application of simplified "desk-top" estimation approaches, or more rigorous and resource intensive in-depth methods such as computerized modeling or additional site monitoring. The goal of this analysis is the generation of quantitative release rate estimates (mass per unit time) for each contaminant release source. The output of this analysis (mass loadings of each contaminant to each environmental medium) serves two distinct but related functions. First, it provides a quantitative basis for comparing the magnitude of various individual on-site releases of each target contaminant. This information will be useful later in the overall site analysis when the cost effectiveness of implementing specific remedial alternatives for individual release sources is considered. Second, it supplies the contaminant release rate values necessary as input for subsequent environmental fate analysis. Individual on-site releases of each contaminant are summed to arrive at 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 short-term release rate will be used in the following environmental fate analysis to project short-term environmental concentrations which, in turn, will be used to estimate short-term (sub-chronic) exposure. Similarly, long-term release rates will be used to project long-term (chronic) concentrations and exposures. When developing the short-term release rate, the analyst should also evaluate and record an associated factor that can be useful when interpreting the short-term exposures that the release rate will be used to develop. Specifically, the frequency of short-term exposure occurrence should be projected. In cases where short-term releases (and associated exposures) occur frequently, the sub-chronic exposure may prove a greater health risk than the long-term intakes. Thus, knowledge of the frequency at which sub-chronic exposure occurs may provide useful insight into the actual degree of sub-chronic risk incurred by receptors.

Simplified quantitative estimation procedures allow release approximation based on chemical- and site-specific factors, and therefore provide more useful results than do approaches based solely on broad assumptions. However, these calculations do not take into account the full range of variables that affect on-site contaminant release. In addition, in all but one case, these approaches assume steady state conditions. That is, 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.* Thus, their utility is constrained, and their application should be limited to the following situations:

(1) Estimation of the level of release of specific contaminants from a site, or from portions of a site. Once major release problems have been identified through the application of these simplified procedures, those release sources of greatest concern can be targeted for an in-depth quantitative analysis (monitoring, modeling).

(2) Projection of the approximate release reduction that can be affected by application of various remedial alternatives. This step provides information for the evaluation of remedial alternatives in the Feasibility Study. Remedial alternatives that clearly do not provide requisite control, as identified via the use of the simplified estimation procedures, can be dropped from further analysis.

In both cases, the use of these procedures supports cost-effective application of resources (time, money, and human resources) to analysis of key issues.

In most cases, the contaminant release calculation procedures presented here relate to the baseline case. However, for air emissions, guidance is provided for use during the Feasibility Study to estimate release rates associated with certain remedial alternatives. In many instances, air releases directly associated with the implementation of a given remedial action will be unavoidable, although such releases would be of short duration, ceasing upon completion of remedial alternative implementation. For water release, while good engineering design should limit additional introduction of contaminants (resulting from the remedial alternative itself) to surface or ground-water systems, the potential for such remediation caused release must be considered. This will require critical review of the remedial alternative design in light

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*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.

of pertinent site characteristics (climatology, hydrology, etc.) and application of engineering judgment and experience with implementation of similar technologies.

Generally, post-remediation contaminant release is estimated by applying the expected level of control associated with a particular option (as determined from the engineering design), adjusted to reflect its expected long-term effectiveness, to the pre-remediation, baseline release value. Note, however, that in the case of volatilization release from landfills, the release estimation equation provided in Section 3.4.2 can be used to directly project the level of release reduction expected with varying remedial design options (i.e., depth and type of landfill soil cover).

Data management forms are presented in Appendix C. These forms may be used to facilitate organization of the results of Level II contaminant release analysis for efficient use in subsequent quantitative contaminant fate analysis (see Chapter 4).

3.4 Atmospheric Contamination

3.4.1 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 the following factors:

(1) Wind erosion of wastes and contaminated soils,

(2) Vehicular traffic movement over contaminated, unpaved roads,

(3) Heavy equipment activity at the site (excavation, loading, etc.),

(4) Incineration of wastes during remediation.

Generally, baseline situations will involve only the first two of these factors. Where there are no anthropogenic or natural controls, fugitive dust generation attributable to these factors will continue over time. In remedial action scenarios, all four factors may contribute to the total fugitive dust load, with remediation-related activity at the site (excavation, vehicular traffic) potentially contributing additional contaminant release to air. However, release of contaminated dust will cease or lessen following remediation, depending on the alternative employed.

(1) Simplified procedures. The procedures that follow are useful in estimating total fugitive dust releases likely to result from the four factors cited above. Once total suspendable dust generation levels have been calculated using these equations, projections of the amounts of hazardous substances expected to enter the atmosphere in fugitive dust can be estimated by either of the following approaches:

- Apply to total dust generation estimates of the percentage by weight of toxic substances in contaminated soil or in disposed wastes. This approach yields estimates of questionable confidence, however, as it does not take into account factors relating to particle size, adsorption potential, etc., that can affect the amount of a contaminant that actually enters the atmosphere as dust.

- Multiply total dust generation estimates by percentages (by weight) of the substances of concern in actual fugitive dust samples obtained via on-site air monitoring. This approach will provide estimates of much higher reliability than those described above, as it inherently takes into account those chemical-specific and site-specific factors that affect release of contaminated dust in the field.

(a) Baseline condition. As previously stated, the total baseline fugitive dust loading will comprise releases due to wind erosion of toxic wastes or contaminated soils, emissions resulting from material excavation, and releases due to vehicular traffic over contaminated areas. Procedures for estimating each of these release sources are discussed below.

Wind erosion.* 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 wind erosion estimation equation that takes this range of variables into account (Skidmore and Woodruff 1968):

$$E = f(I', C', K', L', V) \qquad (3\text{-}1)$$

where

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

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*Applied to non-adhering, non-compacted contaminated soil or waste materials.

These variables are actually aggregate factors that are themselves functions of other variables. Table 3-2 identifies the factors that determine the values of the five variables used in the SCS equation. Directions for applying this equation to a site-specific situation are provided in a series of publications issued by the U.S. Department of Agriculture. 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. These volumes allow each variable required to solve the equation to be accessed via graphs, tables, or nomographs. Thus, once certain site characteristics (e.g., soil particle size range, climate) are known, the equation can be solved. It should be noted, however, that the vegetative cover factor (V) specifically applies to crop residues, and care must be exercised when extrapolating to the cover conditions present at uncontrolled waste sites. Alternatively, for Remedial Investigation and Feasibility Study estimation purposes, a "zero pounds per acre" vegetative cover value may be used. This assumes a worst-case situation (from a vegetation-related wind attenuation perspective) and provides a conservative estimate of contaminated fugitive dust release.

It should also be noted that one need not necessarily investigate site-specific soil properties for a given site in order to obtain requisite variable values for use with the wind erosion equation (or other fugitive dust generation equations). Instead, the necessary soils data can be obtained from the local Soil Conservation Service official. SCS has on record a range of pertinent soils data for sites across the country where soil surveys have been conducted. In addition, the SCS also maintains an extensive computerized soil properties data base called the "Soils 5 File" (soil interpretation records). 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 the 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 facilities or chemical spills. This method uses an emission factor based approach to estimate release and simplified procedures (adapted from existing 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

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Table 3-2. 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)	Fjeld 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.

exposure. Thus, this approach internalizes three key components of exposure analysis: release rate estimation, contaminant migration analysis, and population exposure determination. It should be noted that Cowherd et al. (1985) caution that their method is designed for application to emergency evaluations and should not be used in cases where time is not a limiting factor, except as a preliminary assessment tool used to guide subsequent, more detailed investigation. However, it is felt that the degree of accuracy attainable using this method is consistent with that generally expected to result from simplified quantitative estimation procedures. In addition, this approach directly provides the analyst with estimates of short-term (worst-case, 24-hour) release and exposure estimates, as well as long-term (average annual) estimates. EPA (1983c) defines short-term concentrations to equate with a 10- to 90-day period. Thus, the 24-hour maximum exposure may not adequately represent sub-chronic exposures. On the other hand, the SCS wind erosion equation is designed to provide only annual erosion losses, and cannot be reliably altered to generate short-term estimates.* Therefore, it cannot be used with data delineating climatic extremes for a given location, but must be based on average annual climatic data. Instead, in the analytical procedure presented here, short-term release, estimated using the wind erosion equation, is taken to equal the average release over the first year following site investigation. Long-term release rates are developed through consideration of contaminant loss from the site during the 70-year period upon which long-term chronic exposure estimates are based (see Section 3.4.3).

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

An investigator applies the wind erosion equation via the use of well developed tables, equations, and graphs that are region specific; the equation is therefore easy to use in evaluating given locations across the country. As noted in USEPA (1983a), however, it does exhibit one significant drawback; it computes the total wind erosion soil loss due to the combination of surface creep, saltation, and suspension. Although this is entirely appropriate for studies of agricultural soil loss, for which the equation was developed, in exposure evaluations the analyst is generally concerned only with that fraction of the total soil loss that consists of particles of suspendable, wind transportable, and inhalable size. Thus, when the wind erosion equation is used to estimate

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*Personal communication between Lee Schultz (Versar) and Thomas George (U.S. Soil Conservation Service, (202) 447-6268) July 24, 1985.

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 suspendable and transportable over significant distances by wind. Considerable discussion of the cut-off point for suspendable soil particle size exists in the literature (see Sehmel 1980, Smith 1982, and USEPA 1983a, 1983b). As a group, particles $\leq$ 100 um aerodynamic equivalent diameter include all wind suspendable and transportable particles, and thus encompass inhalable particle sizes (see Miller et al. (1979) for a discussion of the extent to which various particle sizes penetrate the human respiratory system). Of particles within this broad range, those in the 30 to 100 um diameter range will be susceptible to impeded settling within a few hundred feet from the source (USEPA 1983b), while those particles $\leq$30 um in diameter can be transported for considerable distances downwind. For estimation of inhalation exposure, however, only the inhalable fraction of suspended particulates needs to be considered. It is expected that the forthcoming revisions to the national primary air quality standard for particulates will define respirable fraction to equate the particles $\leq$ 10 um in diameter.* Therefore, the 10 um cut-off is used in the following estimation methods.

It has been demonstrated that for particles in the 2 to 20 um 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 $\leq$ 10 um in diameter can be determined based on the soil size distribution of the parent soil. It may 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.

Unpaved roads. The following equation (USEPA 1983b) can be used to estimate fugitive dust releases associated with on-site vehicular traffic on contaminated unpaved roads.

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

or in metric form

$$E_{VT} = k(1.7)\left(\frac{s}{12}\right)\left(\frac{Sp}{48}\right)\left(\frac{W}{2.7}\right)^{0.7}\left(\frac{w}{4}\right)^{0.5}\left(\frac{365-Dp}{365}\right) \qquad (3\text{-}2)$$

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*Personal communication between Gary Whitmyre (Versar) and Kent Berry (Strategy and Air Standards Division, Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, N.C.), July 23, 1985.

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 um (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 3-3).

This emission factor can be applied to "vehicle kilometers traveled per time" values to generate "dust release per time." 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 3-3 reflects the range of average "Dp" values for locations in the U.S. Reduced "Dp" values should be selected in light of the normal value for the site under consideration. 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." 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)
- 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, 1983b), Farino et al. (1983), Sehmel (1980), and Smith et al. (1982).

(b) Remedial action. Fugitive dust releases during remediation can result from a combination of wind erosion and vehicular activity as discussed above, from heavy equipment activity (excavation, loading, etc.), and possibly from implementation of on-site waste incineration. In order to develop quantitative estimates of such releases during remediation, the equations discussed above for wind erosion and vehicular traffic can be used along with the following:

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*See EPA (1983) for "k" values used when release of specific particle size groups other than 10 um is desired.

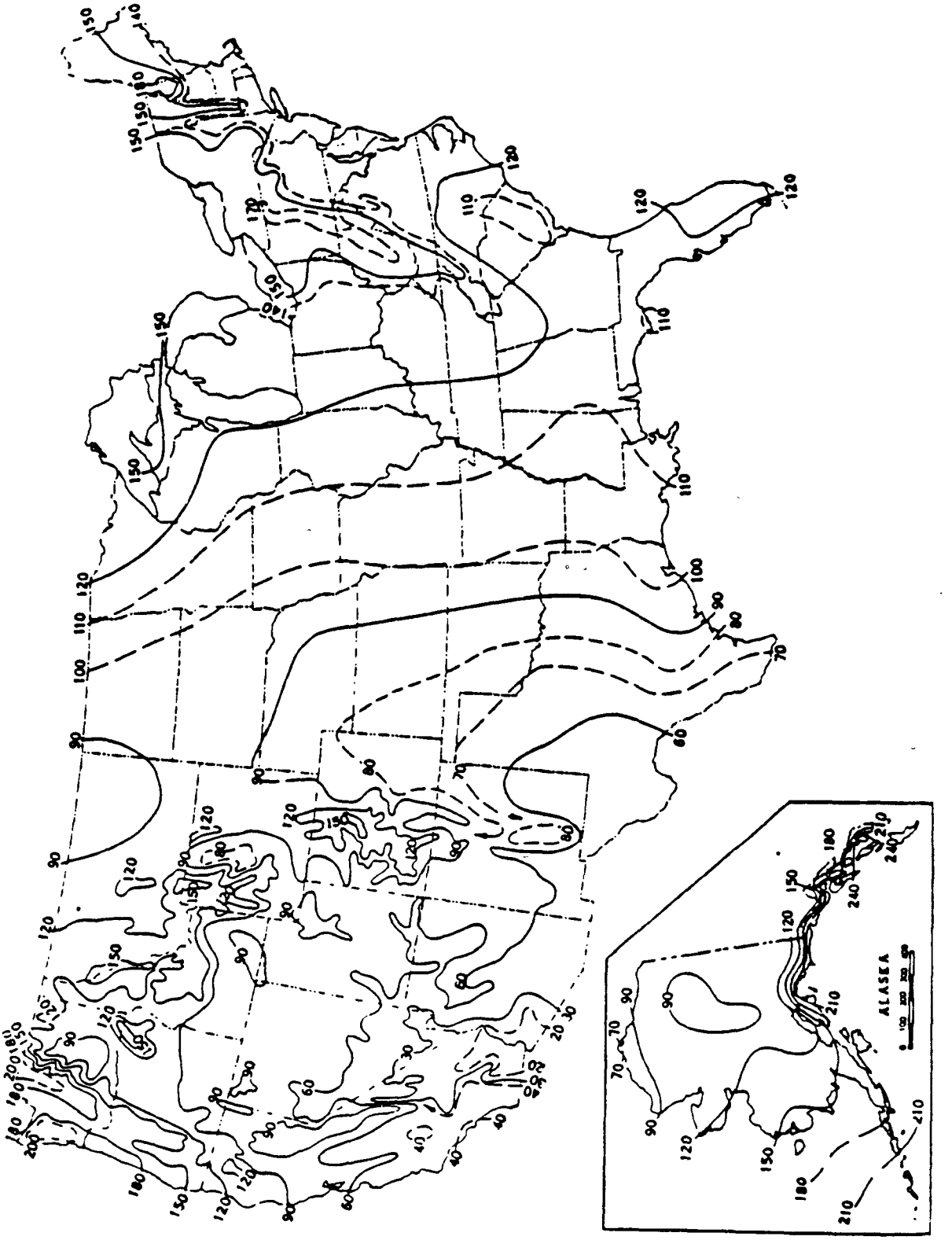

Figure 3-3. Mean Number of Days Per Year with ≥0.01 Inches of Precipitation (i.e., "wet days") (USDC 1968)

Excavation and transfer of contaminated soils. One can use the following equation (USEPA 1983b) to estimate fugitive dust releases resulting from on-site excavation and dumping of contaminated soils.

$$E_{HE} = k(0.0018) \frac{\left(\frac{s}{5}\right)\left(\frac{U}{5}\right)\left(\frac{H}{5}\right)}{\left(\frac{M}{2}\right)^2\left(\frac{Y}{6}\right)^{0.33}}$$

or in metric form

$$E_{HE} = k(0.0009) \frac{\left(\frac{s}{5}\right)\left(\frac{U}{2.2}\right)\left(\frac{H}{1.5}\right)}{\left(\frac{M}{2}\right)^2\left(\frac{Y}{4.6}\right)^{0.33}} \qquad (3\text{-}3)$$

where

E_{HE} = emission factor for heavy equipment (batch dump) operations (lb emission/ton material moved; kg/megagram).
k = 0.36 = particle size multiplier for particles <10 ug.*
s = silt content (of contaminated material), (percent).**
U = mean wind speed, (m/s).
H = drop height, (m).
M = material moisture content, (percent).
Y = dumping device capacity, (m^3).

The equation is designed for application to batch dump material transfer and does not take into account material released to air during excavation. The equation is valid for situations that comply with the following boundary conditions (which must be compared with existing on-site conditions):

- Silt content = 1.3 - 7.3 percent
- Moisture content = 0.25 - 0.70 percent
- Dumping capacity = 2.10 - 7.6 m^3 (2.75 - 10 yd^3)

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*See EPA (1983b) for "k" values used when release of other particle size groups is to be estimated.

**Soil silt content can be estimated from SCS Soils 5 File data (see previous discussion) by subtracting the "percent clay" value from the "percent material passing No. 200 sieve" value. (Personal communication between Keith Young, U.S. Department of Agriculture, Soil Conservation Service, Washington, D.C., and Lee Schultz, Versar Inc., Springfield, Va, May 1, 1984.)

Incineration. In certain cases, on-site incineration of toxic solid wastes may prove a feasible remedial alternative. Although incineration can be effective in destroying toxic substances, it can also result in the release of contaminated particulates. Such release can occur as combustion emissions, or as fugitive emissions from the waste feed system or the incinerator itself. Combustion releases are a function of the waste feed rate, and the system's Destruction and Removal Efficiency (DRE) for specified toxic chemicals in the waste materials. A DRE of 99.99 percent, and thus a combustion release of 0.01 percent, can be assumed based on the requirements of 40 CFR 264.343 (USEPA Regulations for Owners and Operators of Permitted Hazardous Waste Facilities; Subpart O - Incinerators). In order to simplify analysis, fugitive emissions can be assumed to mirror the relative proportions of toxic components in the waste feed. To estimate total particulate emissions from a given incineration option, the analyst should review the proposed system design parameters, as well as the permit operating requirements and pertinent performance standards (i.e., 40 CFR 264.340-345).

(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 provide a quantification of the particulate mass loading attributable to the site alone (assuming that air sampling stations can be sited so as to eliminate interference from other sources). Either simple dispersion equations or computerized air dispersion modeling* can then be exercised to delineate the emission level at a "virtual point source" (i.e., the uncontrolled hazardous waste site) necessary to result in the ambient particulate concentrations observed downwind. 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.

3.4.2 Volatilization Emission Analysis

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

(1) Covered landfills - without internal gas generation;

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*Although computerized dispersion modeling can be used to determine contaminant release rates, it is primarily considered to be a tool for determining contaminant atmospheric fate. Thus, refer to Chapter 4, Environmental Fate Analysis, for detailed discussions of air dispersion models applicable to uncontrolled hazardous waste facilities.

(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. In remedial action scenarios, the above-listed volatilization sources would be controlled, with the degree of control depending on the remedial option or options implemented at the site. In addition, certain remediation alternatives may actually add volatile substances to ambient air, as in the case of air stripping, which removes volatile contaminants from wastewaters by accelerating the volatilization process.

(1) Simplified procedures. This section presents simplified analytical procedures for estimating releases from each of the above source categories. Reductions in volatilization releases associated with any given remedial action 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 cases where a remedial alternative under consideration contributes to volatilization, quantitative projection of the short- and long-term volatilization release must be determined from the engineering design of that remedial action.

Because the volatilization rate is determined primarily by the chemical properties of a given substance, the equations presented here for its estimation require input of quantified property values. These data are available for many chemicals that may be present at uncontrolled hazardous waste sites, and are presented in various chemical reference texts. However, it is also likely that chemicals may be involved for which necessary properties have not been determined. In these cases, 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 pertinent reference materials such as Lyman et al. (1982). In addition, readily accessible computerized systems are available to predict a range of pertinent chemical properties. For example, the computerized Graphic Exposure Modeling System (GEMS), and its subsystem CHEMEST, provides one such tool. This system has been developed and is managed by the EPA Office of Toxic Substances in Washington, D.C. It is essentially a

computerized version of Lyman et al. (1982), and can be rapidly accessed for estimation of 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 comprehensive survey of available air release models for volatile substances and a critical analysis of the applications and limitations of each. The volatilization release estimation equations contained in the following subsections were determined by Farino et al. to constitute those most suitable for such analysis.

(a) Baseline condition

Landfills without internal gas generation. The equation cited below (i.e., Equation 3-4) can be used to estimate volatilization releases from covered landfills containing toxic materials alone, or toxic materials segregated from other landfilled non-hazardous wastes. Equations 3-5 through 3-8 are provided to allow calculation of certain input variables that are required to apply Equation 3-4. Farmer et al. (1978) developed an equation for estimating the effectiveness of various landfill cover types and depths in controlling volatilization release. 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. Thus, diffusion of the toxic vapor through the soil cover is the controlling factor.

This equation was simplified by Farmer et al. (USEPA 1980b) by incorporation of 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 calculation of 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 also 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 and Farino et al. (1983) is:

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

where

E_i = emission rate of component i, (g/sec).
D_i = diffusion coefficient of component i, (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).
d_{sc} = effective depth of soil cover, (cm).
M_i = mole fraction of toxic component i in the waste, (g/g).

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 of water adhering to soil particles), thereby effectively increasing the vapor path (USEPA 1980b). Farmer et al. suggest however, that when using their equation for designing 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 3-4. It is recognized, however, that situations may exist 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 (P_a) may be more appropriate, and this value may be substituted for P_t in Equation 3-4 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):

$$D_i = \frac{0.001T^{1.75}\sqrt{\frac{1}{MW_i} + \frac{1}{MW_a}}}{P_a[(\Sigma V_i)^{1/3} + (\Sigma V_a)^{1/3}]^2} \qquad (3\text{-}5)$$

where

T = absolute temperature, (°K).
MW_i;MW_a = molecular weights of toxic substance and air (28.8), respectively, (g/mole).

$\Sigma V_1; \Sigma V_a$ = 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).

P_a = absolute pressure, (atm).

For estimation of short-term (maximum) release rates, use a value for temperature that reflects expected summer maximum temperatures. Annual average temperatures should be used to initially estimate long-term (average) release rates. Note, however, that this initial estimated long-term release value will be revised as described in Section 3.4.3 to develop final long-term release estimates.

Relevant atomic diffusion volumes for use in estimating D_1 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 3-3 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_1 involves the identification of a compound listed in Table 3-3 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:

$$D_1 = D'\left(\frac{MW'}{MW_1}\right)^{1/2} \qquad (3\text{-}6)$$

where

D_1 = diffusion coefficient of the compound to be estimated from the known D'.

MW_1 = molecular weight of the compound to be estimated.

D' = diffusion coefficient of a compound that can be found in the table, the molecular weight and molecular diffusion volume of which are close to that of the unknown.

MW' = molecular weight of the selected compound D'.

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

*This value is from Shen (1981).

Table 3-3. 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

Table 3-3. (continued)

Compound	Formula	Molecular weight	Atomic diffusion volume	Diffusion coefficients (cm^2/sec) at 10°C	at 30°C	at 50°C
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	114.96	.06858	.07729	.08643
Tetrachloroethylene	C_2Cl_4	166	111.00	.06968	.07852	.08781
Toluene	C_7H_8	92	111.14	.07367	.08301	.09283
Trichloroethane	$C_2H_3Cl_3$	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

$$P_t = 1 - \frac{\beta}{\rho} \qquad (3\text{-}7)$$

where

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 is used for most mineral material.

For estimation, P_t can be assumed to be approximately 0.55 for dry, non-compacted soils, and approximately 0.35 for compacted soils. This same value (0.35) is also appropriate for use as a generic air filled soil porosity (P_a) when analyzing 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 (Farmer 1980b):

$$C_{si} = \frac{pMW_i}{RT} \qquad (3\text{-}8)$$

where

p = vapor pressure of the chemical,** (mm Hg)
MW_i = mole weight, (g/mole).
R = molar gas constant, (62.3 mm Hg/°mole).
T = absolute temperature, (K).

Again, use maximum summer temperatures to estimate short-term release and annual average temperatures to initially estimate long-term release. See Section 3.2.3 for directions for calculating a final long-term release rate.

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 which, due to their considerable organic content, generate landfill gases (e.g., H_2, CH_4, CO_2). In such cases, the upward movement (convective sweep) of the landfill gas becomes

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*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).

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 effect of the landfill gas is so great that both soil and gas phase diffusion become essentially insignificant. Thus, the following simplified equation is recommended for estimating volatilization of toxic substances from co-disposal landfills:

$$E_i = C_i^* V_y A \qquad (3\text{-}9)$$

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. However, it is noted in Thibodeaux (1981) that various site factors such as the presence of saturated soils will tend to reduce the rate of volatile chemical release from landfills. Therefore, 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.

Spills, leaks. Equations 3-10 and 3-12 will estimate volatilization release from fresh and old (respectively) chemical spills on soil. Equations 3-11 and 3-13 through 3-15 provide means of estimating certain input variables required to solve Equations 3-10 and 3-12.

As discussed in Farino et al. (1983), one can apply Equation 3-10 (adapted from Thibodeaux and Hwang 1982) to estimate volatilization 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:

$$E_i = k_{iG}\, C_i{}^{*} A \qquad (3\text{-}10)$$

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.

$$k_{iG} = \left(\frac{MW_{H_2O}}{MW_i}\right)^{0.335} \left(\frac{T}{298}\right)^{1.005} \left(k_{iG,H_2O}\right) \qquad (3\text{-}11)$$

where

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

For 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 3.4.3.

In cases where past spills, leaks, or intentional disposal directly onto or into surface soils (landfarming) have resulted in contaminated surface soils, Equation 3-12 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. The equation as originally presented in Thibodeaux and Hwang (1982) was designed for application to active or planned landfarms for petroleum wastes. It has been determined (Farino et al. 1983) 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. Note, however, that use of this equation is inherently limited to situations where there indeed exists a discernible dry zone at the surface of the contaminated soil. 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).

$$E_i = \frac{DC_sA}{\sqrt{d^2 + 2Dt}} \qquad (3\text{-}12)$$

where

E_i = emission rate of component i, (g/sec).
A = contaminated surface area, (cm^2).
C_s = the liquid-phase concentration of component i in the soil, (g/cm^3).
t = time measured from sampling time, (seconds).
d = depth of dry zone at sampling time, (cm).

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:

$$D = D_i P_t^{4/3} H_i' \qquad (3\text{-}13)$$

where

D_i = diffusion coefficient of component i, (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 3-4 for a discussion of the application of and values for these two terms.

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):

$$H_i' = \frac{H_i}{RT} \qquad (3\text{-}14)$$

where

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

Again, use summer maximum temperatures for estimation of short-term release and annual average temperatures for initial estimation of long-term release. Final long-term release rates are developed as discussed in Section 3.2.3.

Note that Equation 3-12 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:

$$t_d = \frac{h^2 - d^2}{2D} \qquad (3\text{-}15)$$

where

h = depth from soil surface to the bottom of the contaminated region, (cm).

Lagoons. Mackay and Leinonen (1975) have developed an equation for estimating volatilization releases of low solubility compounds from water bodies such as hazardous waste lagoons. This is presented as Equation 3-16. Equations 3-17 and 3-18 provide means of calculating certain input parameters required by Equation 3-16. 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):

$$E_i = K_i C_s A \qquad (3\text{-}16)$$

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:

$$\frac{1}{K_i} = \frac{1}{k_{iL}} + \frac{RT}{H_i k_{iG}} \qquad (3\text{-}17)$$

where

k_{iL} = liquid phase mass transfer coefficient, (cm/sec). See Equation 3-18.
k_{iG} = gas phase mass transfer coefficient, (cm/sec). See Equation 3-11.
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).

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:

$$k_{iL} = \left(\frac{MW_{O_2}}{MW_i}\right)^{0.5} \left(\frac{T}{298}\right) \left(k_{L,O_2}\right) \qquad (3\text{-}18)$$

where

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

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).

(b) Remedial action. Waste treatment processes used as part of a remediation strategy can themselves contribute significant releases of volatile materials to the ambient air. Stripping of volatiles from

wastewaters, for example, generally involves artificial acceleration of the natural volatilization process, thereby resulting in forced transfer of the volatile contaminants from wastewater to air. Generally, users must evaluate the engineering design of each remedial alternative under consideration to determine the level of toxic vapor release associated with its implementation. The user of this manual is referred to Farino et al. (1983) for a discussion of wastewater treatment air emission estimation methods. For incineration of toxic wastes, a Destruction and Removal Efficiency (DRE) of 99.99 percent, and thus a release of 0.01 percent, can be assumed, based on the requirements of 40 CFR 264.343 (Environmental Protection Agency Regulations for Owners and Operators of Permitted Hazardous Waste Facilities; Subpart O - Incinerators).

(2) In-depth analysis. In-depth analysis of volatilization 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 4 of this manual for a detailed description of air contaminant dispersion modeling tools.

3.4.3 Long-term and Short-term Release Calculation

Long-term release values (70 years) for wind erosion of contaminated particulates, and for volatilization from landfills with and without internal gas generation, spills, and lagoons can be estimated as follows:

$$E_{Ai} = \frac{V_c C_i}{70} \; 1 - e^{-\frac{E}{V_c C_i}(2.2\times10^9)} \qquad (3\text{-}19)$$

where

E_{Ai} = average annual release of contaminant i, (g/yr).
V_c = volume of contaminated region, (cm^3).
C_i = concentration of contaminant i, (g/cm^3).
E = total 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 to mass per second by dividing by 3.16×10^7 seconds.

To estimate long-term release from contaminated surface soils, Equation 3-15 (converted to years by dividing by 3.16×10^7) 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 it is expected that some contaminant will remain after 70 years (i.e., $70 < t_d$), use the following equation to estimate long-term release:

$$E_{Ai} = \frac{AC_s}{70}[(d^2 + 4.4 \times 10^9 D)^{1/2} - d] \qquad (3\text{-}20)$$

where

- 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 = relates the amount of contaminant that goes from liquid to gas phase, and then from gas phase to diffusion in air (see Equation 3-13).

Note that this approach does not include consideration of contaminant loss due to chemical degradation, and is thus 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 and breezy conditions can significantly accelerate the rate of volatile release, while high winds alone can greatly increase the amount of contaminated particulate matter being blown from the site. However, such mechanisms also provide greater dilution of the contaminants. Thus, the mechanisms that are capable of generating the maximum contaminant release may not equate with conditions most conducive to maximum environmental concentrations and associated human exposure. Therefore, using the appropriate (maximizing) input parameters provided in previous sections, short-term maximum contaminant release is defined as that level of release calculated for release events during the first year period following site investigation.

The above approach to estimation of 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 4).

3.5 Surface Water Contamination Analysis

Contaminated runoff, as well as overland flow of toxic contaminants from storage leaks and spills or from lagoon failures, will generally constitute the surface water contamination sources of concern at uncontrolled hazardous waste sites. 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. This section discusses methods for quantifying toxic releases of uncontrolled hazardous waste sites to surface water bodies.

3.5.1 Simplified Procedures

(1) Baseline condition. A large proportion of the types of organic substances of concern found at Superfund sites are relatively non-polar, hydrophobic substances (Delos et al., 1983). 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.

(a) Soil loss calculation. The basic equation for estimation of soil loss is presented as Equation 3-22. Equations 3-23 through 3-26 are provided to guide calculation of certain input parameters required to apply Equation 3-22. The modified universal soil loss equation (Williams 1975) as presented in Mills et al. (1982) is:

$$Y(S)_E = a(V_r \cdot q_p)^{0.56}\ KLSCP \qquad (3\text{-}21)$$

where

$Y(S)_E$ = sediment yield (tons per event, metric tons).
a = conversion constant, (95 English, 11.8 metric).*

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

V_r = volume of runoff, (acre-feet, m^3).
q_p = peak flow rate in cubic feet per second, (m^3/sec).
K = the soil-erodibility factor, commonly expressed in tons per acre per R unit.
R = the rainfall factor, expressing the erosion potential of average annual rainfall in the locality, (both K and R 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).

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

$$V_r = aAQ_r \tag{3-22}$$

where

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

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

$$Q_r = (R_t - 0.2S_w)^2/(R_t + 0.8S_w) \tag{3-23}$$

where

Q_r = the depth of runoff from the watershed area, (in, cm).
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):

$$S_w = \left(\frac{1000}{CN} - 10\right) a \tag{3-24}$$

where

CN = the SCS Runoff Curve Number (dimensionless, see Table 3-4).
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 values of uncontrolled hazardous waste sites from Table 3-4.

Table 3-4. 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 = 8-12mm/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 = 1-4mm/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.

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

$$q_p = \frac{aAR_tQ_r}{T_r(R_t - 0.2S_w)} \qquad (3\text{-}25)$$

where

q_p = the peak runoff rate, (ft^3/sec, m^3/sec).
T_r = storm duration, (hr).
a = conversion constant, (1.01 English, 0.028 metric).

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 3-4 through 3-6. The cover management factor, C, is determined bv the amount and type of vegetative cover present at the site. Its value is "1" (one) for bare soils. Consult Tables 3-5 and 3-6 to obtain C values for sites with vegetative covers. The factor P refers to any erosion control practices that may be 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.

(b) Dissolved/sorbed contaminant loading calculation. As discussed in Mills et al. (1982), with the following equations the analyst can predict the degree of soil/water partitioning expected for given compounds once storm event soil loss has been calculated. First, the amounts of adsorbed and dissolved substance are determined, using the equations presented below (Haith 1980):

$$S_s = [1/(1 + \theta_c/K_d\beta)]\ (C_i)\ (A) \qquad (3\text{-}26)$$

and

$$D_s = [1/(1 + K_d\beta/\theta_c)]\ (C_i)\ (A) \qquad (3\text{-}27)$$

where

S_s = sorbed substance quantity, (kg, lb).
D_s = dissolved 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).

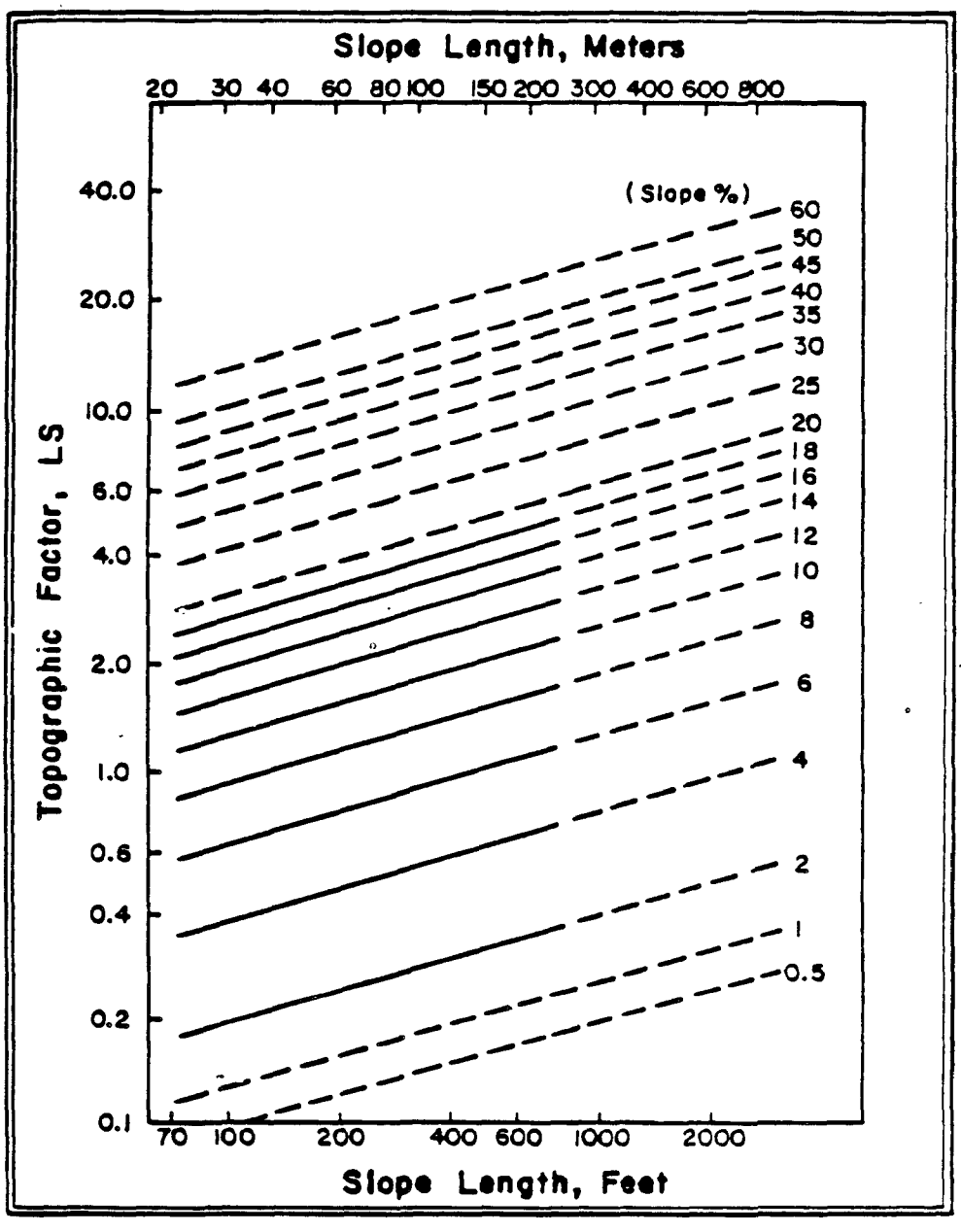

Figure 3-4. Slope Effect Chart Apnlicable to Areas A-1 in Washington, Oregon, and Idaho, and All of A-3: See Figure 3-5 (USDA 1974)

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

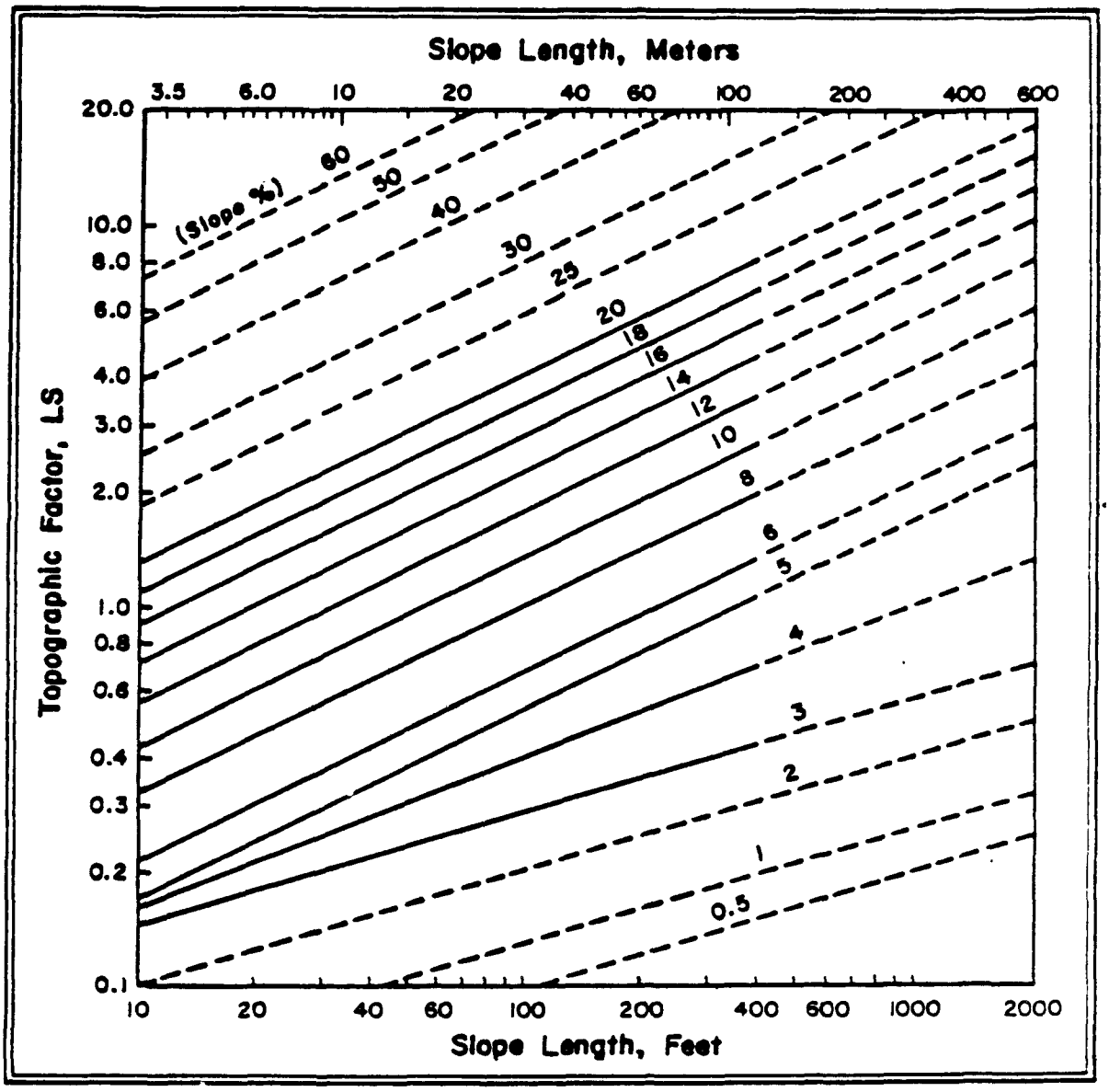

Figure 3-5. Slope Effect Chart for Areas Where Figure 3-5 Is Not Applicable. (USDA 1974)

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

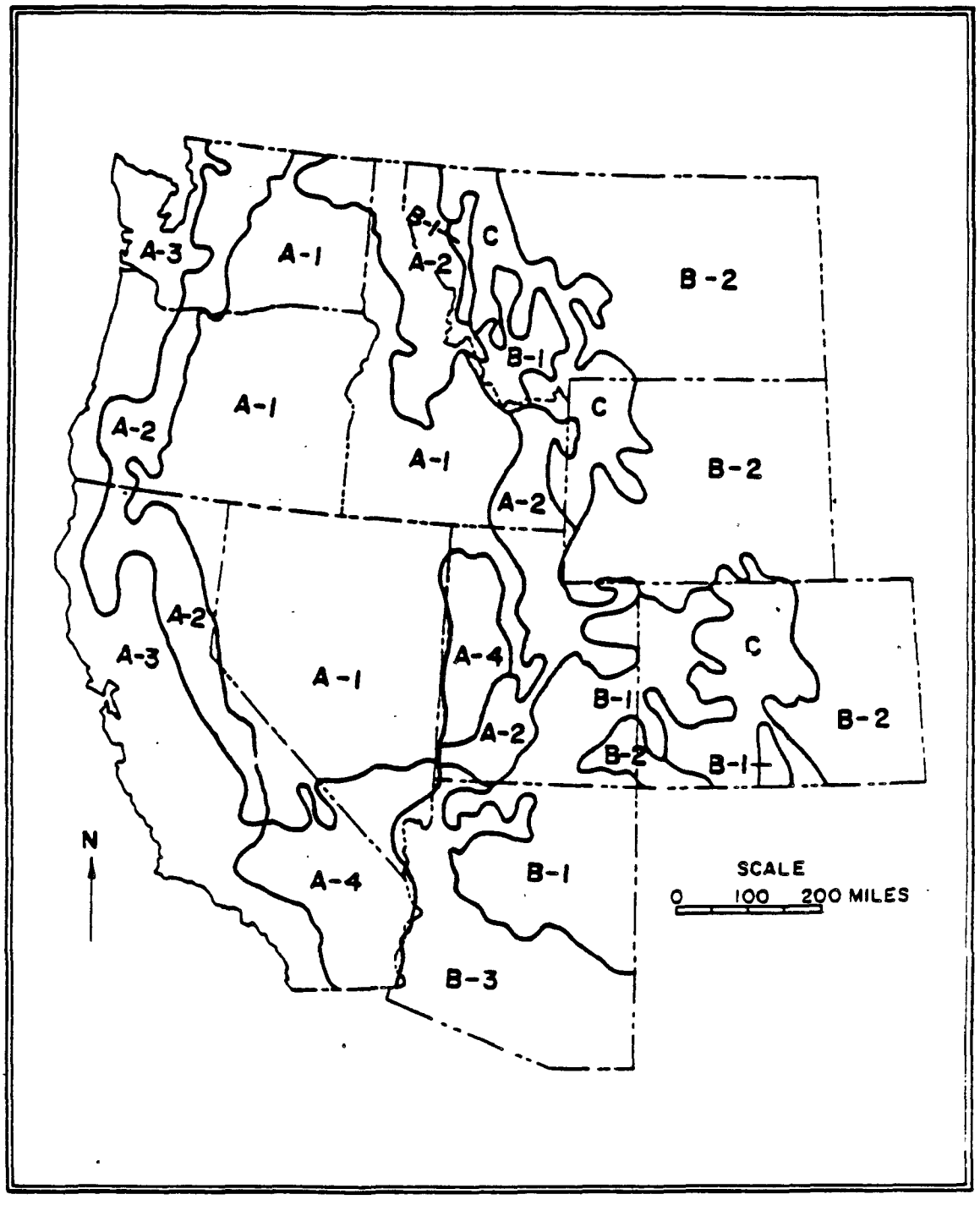

Figure 3-6. Soil Moisture-Soil Temperature Regimes of the Western United States. (USDA 1974)

Table 3-5. "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						
			Percent ground cover					
		Type[d]	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	0.36	0.17	0.09	0.038	0.012	0.003
		W	0.36	0.20	0.13	0.082	0.041	0.011
	50	G	0.26	0.13	0.07	0.035	0.012	0.003
		W	0.26	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 3-6. "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	70-40	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.

β = soil bulk density, (g/cm^3).
C_i = total substance concentration, (kg/ha, lb/acre).
A = contaminated area, (ha, acre).

This model assumes that only that 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 bioconcentraton 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 loading to the receiving water body is calculated as follows (Haith 1980):

$$PX_i = [Y(S)_E/100\ \beta]\ S_s \qquad (3\text{-}28)$$

and

$$PQ_i = [Q_r/R_t]\ D_s \qquad (3\text{-}29)$$

where

PX_i = sorbed substance loss per event, (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).

PX_i and PQ_i can be converted to mass per volume terms for use in estimating contaminant concentration in the receiving water body by multiplying by the site area and dividing by the site storm runoff volume (V_r, see Equation 3-23).

(2) Remedial action. Although remedial technologies implemented at Superfund sites will be designed to preclude continuing contaminant release over time, insofar as is possible, the likelihood of control

failure must still be evaluated. For example, under RCRA regulations, run-on/run-off controls designed for a 25-year storm event are required. However, it can be estimated that there is a 94 percent probability of exceeding a 25-year storm event over a 70-year period.* From this example it can be seen that the possibility of episodic releases at some sites may be high and would, therefore, require careful evaluation. Such evaluation can be considerably facilitated by the use of modeling techniques appropriate for the remedial technologies under consideration. USEPA (1985e) provides considerable guidance on the application of numerical modeling in evaluating the expected degree of effectiveness of remedial alternatives in controlling overland runoff-related contaminant release from hazardous waste sites.

3.5.2 In-depth Analysis

(1) Baseline condition. Releases to surface water bodies at uncontrolled hazardous waste sites can most accurately be quantified 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 4) can be used to "back up" the measured ambient concentration to the "virtual point source."

(2) Remedial action. As stated above, the potential for episodic releases during the 70-year (long-term) time frame must be evaluated on a case-by-case basis.

3.5.3 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.

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*Information provided by Kevin Garrahan, Exposure Assessment Group, Office of Research and Development, U.S. Environmental Protection Agency.

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

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

$$E_{Ai} = BN \qquad (3\text{-}30)$$

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 3-29 and 3-30).
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 3-22) 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:

$$Y(S)_A = R_r KLSCP \qquad (3\text{-}31)$$

where

$Y(S)_A$ = Annual soil loss in runoff
R_r = Rainfall and runoff factor (dimensionless).

Other variables are as defined for Equation 3-22. Note that in certain areas of the Pacific Northwest and central western states, thaw and snowmelt may contribute the majority 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).

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*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.

- Based on the average contaminant concentration in site soils, 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 to 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 associated steady-state runoff effluent 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.

It is recognized that many factors influence the actual degree of contaminant loss in given storm events. Because of the great variety in such factors from locale to locale, no single method will guarantee accurate estimates of short-term contaminant losses in runoff from all sites. However, it is felt that 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 considered to be too ephemeral to adequately reflect short-term releases as defined herein (i.e., 10-90 days). Therefore, a storm event that will generate contaminant releases adequate to affect water quality over a time period approaching the ten-day lower bound of the short-term time frame is needed. For this analysis, a 1-year, 24-hour storm event has been selected. Data quantifying the amount of rainfall that corresponds with the 1-year, 24-hour storm event (as well as similar data for other storm return periods and durations) are provided in USDC (1961).

The user of this manual should note that, based on the work of Haith et al. 1980, research is presently underway at Cornell University*

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

to develop runoff loading factors for organic chemicals in soils. After these are developed, the analyst will be able to obtain average loading values based simply on a chemical's octanol/water partition coefficient and the geographic location under study. This will greatly simplify generation of long-term average release estimates. It is projected that this data base, which will not address short-term extreme events, should be developed by December 1986.

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 4, Environmental Fate Analysis.

3.6 Ground-water Contamination Analysis

Ground-water contamination at uncontrolled hazardous waste sites results from leaching of toxics from contaminated surface or subsurface soils, and from seepage of concentrated contaminants from lagoons and ponds. Approaches exist for both direct and indirect evaluation of the degree and extent of such contaminant release to ground water. This section addresses these methods.

3.6.1 Simplified Procedures

(1) Baseline condition. A method has recently been published that is designed to support rapid (within a 24-hour period) estimation of the level of ground-water contamination attributable to toxic contamination situations. Based on the critical site- and chemical-specific characteristics listed in Table 3-7, this approach relies on the use of tables and nomographs for the estimation of contaminant release and loading to an aquifer. The method is specifically designed to analyze abandoned hazardous waste sites (as well as spills), although it provides only order-of-magnitude estimates of contaminant loading to the saturated-zone (aquifer). In addition, proper application of the method requires a sound background in related scientific/engineering fields, such as hydrogeology and soil science. Refer to Donigian et al. (1983) for a complete description of this analytical method, as well as its applications and limitations.

(2) Remedial action. 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 in the event of an unexpected spill of toxics during implementation of the remedial action, contaminant release should be slow enough to allow spilled substances to be isolated prior to their reaching the saturated zone. Contaminant release control effectiveness, however, may

Table 3-7. Critical Compound and Site Characteristics

Critical Compound Characteristics

1. Contaminant identity and physical state
2. Extent of the contamination
3. Solubility
4. Adsorption
5. Degradation
6. Toxicity
7. Concentration and loading
8. Density, viscosity, and temperature

Critical Site Characteristics (Applicable to both the unsaturated and saturated zones unless otherwise indicated)

1. Identity of subsurface medium
2. Age of site
3. Distances to wells, streams, property boundaries
4. Porosity
5. Infiltration, net recharge, and volumetric water content (unsaturated zone only)
6. Bulk density
7. Hydraulic conductivity (saturated zone only)
8. Chemical characteristics of medium
9. Dispersion
10. Depth to ground water (unsaturated zone only)
11. Hydraulic gradient (saturated zone only)
12. Effective aquifer thickness (saturated zone only)
13. Structural and geologic features

Source: Donigian et al. 1983.

vary among potentially useful remediation technologies. For evaluation of post-remediation control effectiveness, the analyst is referred to USEPA (1985e) for a detailed discussion of both simplified methods and numerical modeling approaches to such analysis.

3.6.2 In-depth Analysis

(1) Baseline condition. In-depth analytical approaches for quantification of baseline contaminant release to ground water involve use of computerized models. Refer to Chapter 4 of this manual for a detailed discussion of the nature and applications of such modeling tools.

(2) During remediation. As stated above, well-designed remedial alternatives would be expected to preclude the potential for remediation-related ground-water contamination. The analyst is again referred to USEPA (1985e) for a discussion of computerized modeling techniques useful in assessing post-remediation contaminant release control effectiveness.

3.6.3 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 3.4.3).

3.7 Soil Contamination

Surface soils at uncontrolled hazardous waste sites may become contaminated with toxic materials through intentional placement of wastes on the ground (dumping, landfarming), as a result of spills, as a consequence of lagoon failure (overland flow), or as a result of contaminated site runoff. Leaching of toxics from a contaminated soil surface can carry contaminants into subsurface layers. Generally, the substances of concern at uncontrolled hazardous waste sites are non-polar (Delos et al. 1983) and will bond (adsorb) strongly to organic soil particles as a result of their hydrophobic properties.

3.7.1 Simplified Procedures

(1) Baseline condition. No estimation methods are presented for surface soils, since site soils will be sampled directly and the degree and extent of their contamination delineated during the Remedial Investigation. For subsurface soils, sampling and analysis may also have been conducted. However, in certain cases it may be desirable to project subsurface contamination without conducting unsaturated zone sampling.

As discussed previously, Donigian et al. (1983) have recently published an analytical method that is specifically designed for such evaluation. This approach, based on the use of tables and nomographs developed to allow rapid estimation of contaminant movement, provides quantitative estimation of subsurface soil contamination.

(2) During remediation. Additional contamination of soils can probably be avoided by well-engineered remedial alternatives. However, in some circumstances, short-term ancillary soil contamination may be unavoidable, as when toxics containment vessels rupture unexpectedly during handling. Estimation of the level of additional remediation-related soil contamination must be made on a case-by-case, best judgment basis, considering the nature and condition of toxics placement at the site and the engineering design of the remedial alternative(s) under consideration.

3.7.2 In-depth Analysis

(1) Baseline condition. Surface soil monitoring, usually conducted during the Remedial Investigation as mentioned above, constitutes in-depth quantitative analysis. Subsurface (unsaturated zone) in-depth analysis will usually involve application of sampling and modeling approaches. Sampling and analysis can provide a direct quantification of the degree of contamination in subsurface soils. Alternatively, computer models exist (e.g., SESOIL, see Bonazountas and Wagner 1981) that are capable of projecting the level of unsaturated zone contamination over time from surface placement of toxics. Refer to Chapter 4 of this manual for a detailed discussion of computer models that can be applied to unsaturated zone contamination estimation.

(2) During remediation. Well engineered remedial alternatives would be expected to correct rather than cause soil contamination on site. However, as discussed above, short-term, remediation related soil contamination may be unavoidable under certain circumstances. No quantitative analysis method is presented for surface soil, however, because remediation related contamination of the surface would have to be estimated on a case-by-case basis from site conditions and engineering design.

3.7.3 Long-term and Short-term Release Calculation

The potential for post-remediation long-term or short-term soil contamination must be evaluated on a case-by-case basis. Such contamination would be associated with failure of an on-site containment remediation technology. Also, as discussed above, short-term soil contamination may result from implementation of the remedial alternative itself. The likelihood of this must also be evaluated on a case-by-case basis in light of site conditions and the design of the selected remedial alternative.

4.0 ENVIRONMENTAL FATE ANALYSIS

4.1 Introduction

Environmental fate analysis assesses the areas affected by, and estimates the concentrations of, hazardous substances released to the ambient environment. Qualitative release assessments, or quantitative release rate estimates derived from the steps described in the preceding chapter, provide the basis for this analysis. For each released contaminant in each receiving medium, various environmental transport, transformation, and removal mechanisms are considered or quantified. The results of fate assessment subsequently support identifying populations exposed to contaminants in the ambient environment, and assessing exposure levels (Chapters 5 and 6).

This chapter provides decision networks and guidance for qualitative screening of environmental fate pathways and an overview of applicable quantitative techniques. Simplified algorithms for estimating ambient contaminant concentrations based on the most important fate mechanisms are presented, and annotated lists of more sophisticated methods and computer-based models are presented for each environmental medium.

4.2 Environmental Fate Screening

Environmental fate screening provides an initial qualitative assessment of contaminant migration or transport in the environment and of the likely ambient contaminant concentration ranges at affected locations. The starting point of this assessment is the results of the contaminant release screening assessment; the fate of each potential release thus identified is systematically assessed in each environmental medium.

In the following subsections, decision networks are presented as a framework for environmental fate screening assessments. Each subsection is keyed to points within the accompanying decision networks and provides additional detail about individual steps.

In each of these networks, certain negative decisions result in the elimination of a given fate pathway as resulting in potentially significant ambient environmental concentrations. These are represented in each case by a box containing the word "No." Such decisions indicate that further assessment is unnecessary.

When positive responses to successive decision points determine that significant ambient concentrations are likely to result from a given pathway, a qualitative screening assessment of human exposure and an identification of exposed populations must be made. Procedures for screening assessments of exposed populations are presented in Chapter 5, Identification of Exposed Populations.

In cases where available site survey data include the results of sampling and analysis of surrounding ambient environmental media, these data may form the basis of environmental fate screening assessments or may provide enough data in themselves so that no further assessment need be undertaken. The media and locations sampled should be compared with the expected extent of contaminant migration, and procedures outlined below should be employed to fill data gaps and to project future trends.

4.2.1 Contaminant Environmental Fate Screening: Atmospheric Fate

The following numbered paragraphs are provided to facilitate interpretation and application of the atmospheric fate decision network presented as Figure 4-1. Each paragraph refers to a particular numbered box in the figure.

1. Atmospheric fate of contaminants must be assessed whenever it is determined that significant gaseous or airborne particulate contaminants are released from the site. In addition, 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. 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). Off-site areas affected by ambient concentrations of gaseous contaminants are determined by atmospheric stability and wind speeds. 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, while low stability or high wind speed conditions cause greater dispersion and dilution of contaminants, resulting in lower concentrations over greater 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 also cause particulates to remain airborne longer (which may also increase release rates). Low winds and high stability

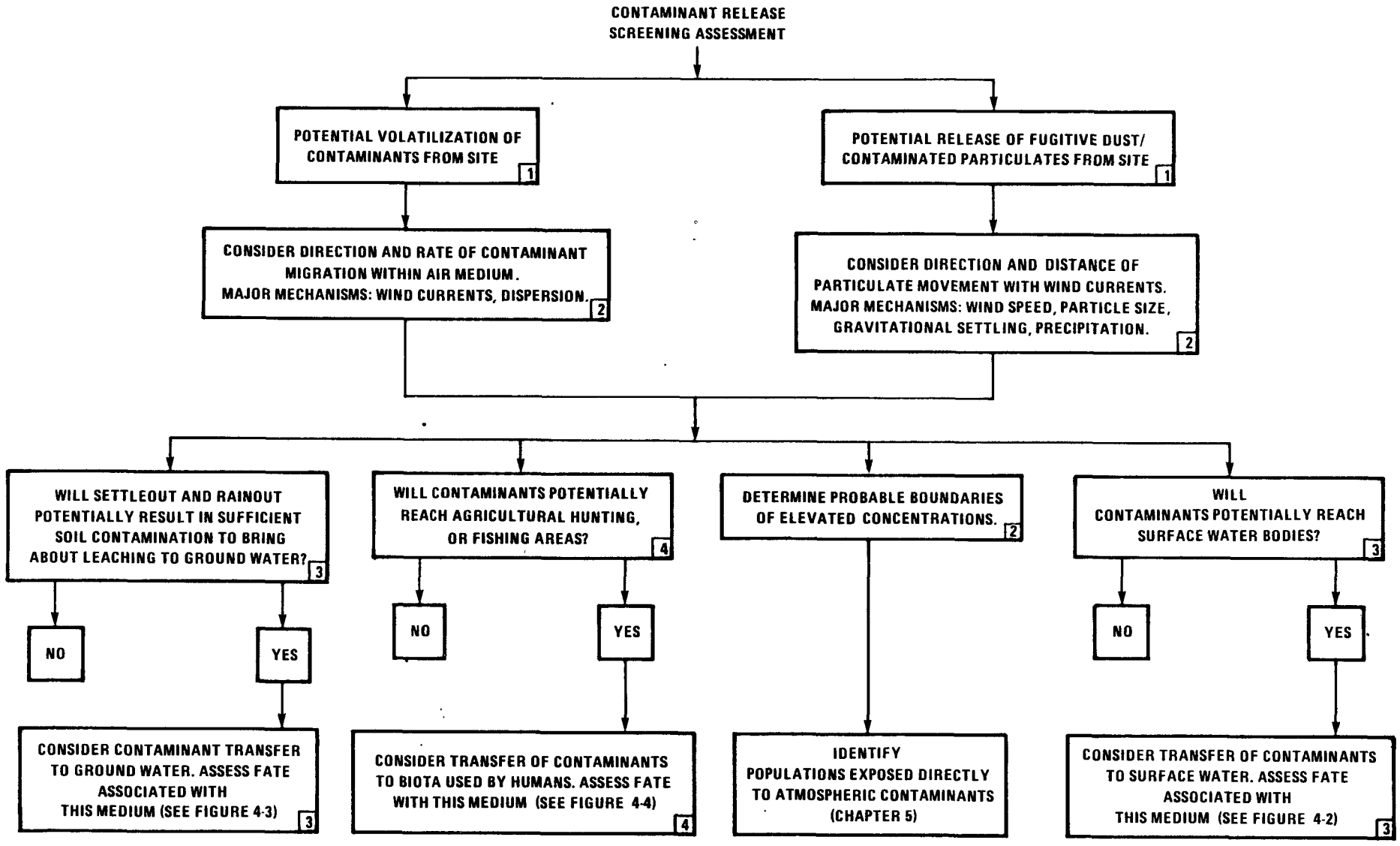

FIGURE 4-1. ENVIRONMENTAL FATE SCREENING ASSESSMENT DECISION NETWORK: ATMOSPHERE

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 due to 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 rain water 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 it is determined that such intermedia transfers are likely, the fate of contaminants in the receiving media should be assessed.

4. If areas identified as likely to receive significant atmospheric contaminant concentrations include areas supporting edible biota, the bio-uptake 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.

4.2.2 Contaminant Environmental Fate Screening: Surface Water Fate

The following numbered paragraphs are provided to facilitate interpretation and application of the aquatic fate decision network presented as Figure 4-2. Each paragraph refers to a particular numbered box in the figure.

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.

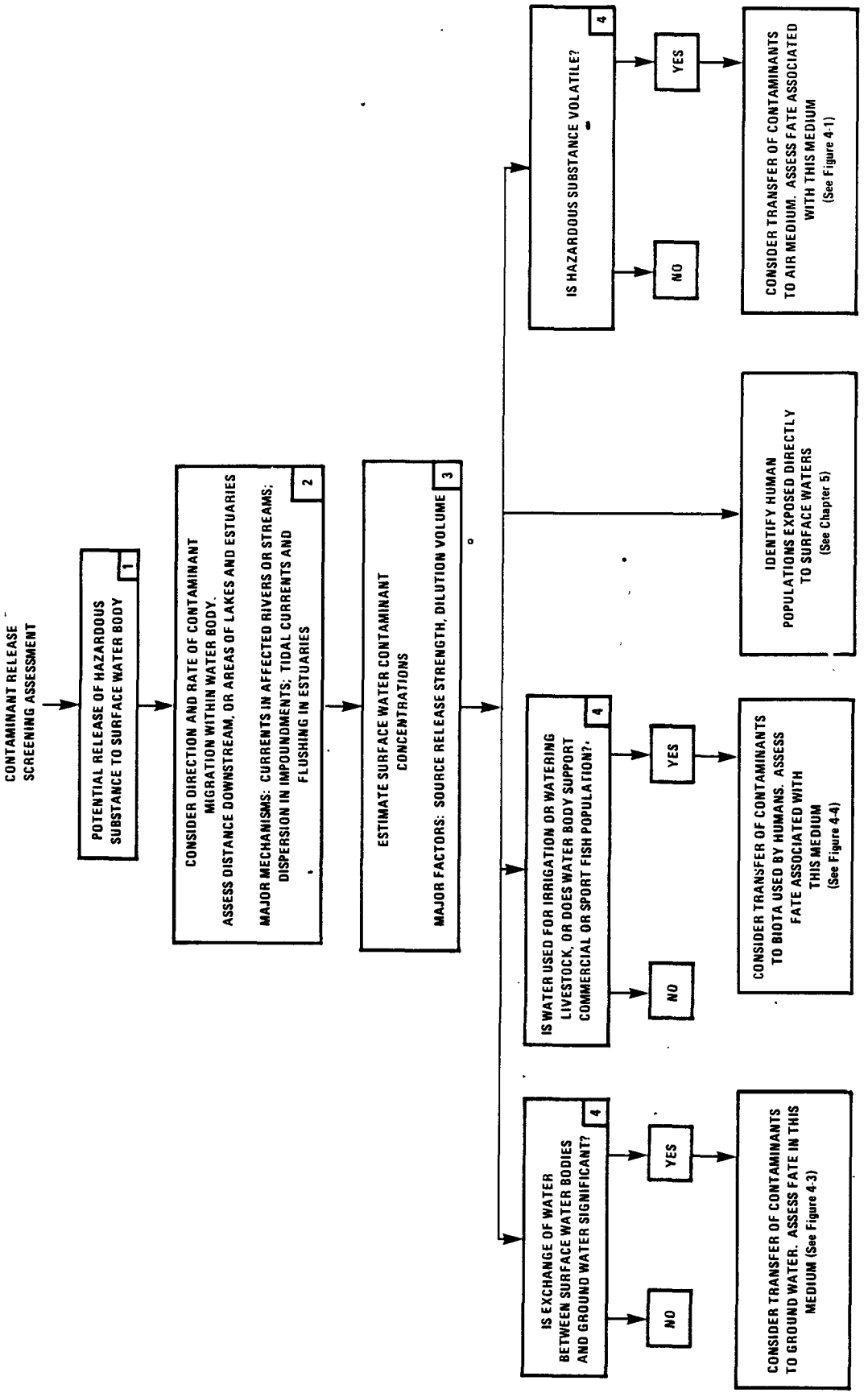

FIGURE 4-2. ENVIRONMENTAL FATE SCREENING ASSESSMENT DECISION NETWORK: SURFACE WATER

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 water bodies. In most cases, entire water bodies 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 water bodies.

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. Again, the conservative approach is to schedule such water bodies receiving significant amounts of contaminants for 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 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 adsorb to 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 inter-association. 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.

4.2.3 Contaminant Environmental Fate Screening: Soil and Ground-water Fate

The following numbered paragraphs are provided to facilitate interpretation and application of the soil and ground-water fate decision network presented as Figure 4-3. Each paragraph refers to a particular numbered box in the figure.

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

2. 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 assessments 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 unreliabile 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) provides a more reliable basis for contaminant transport assessment than do surface topographs.

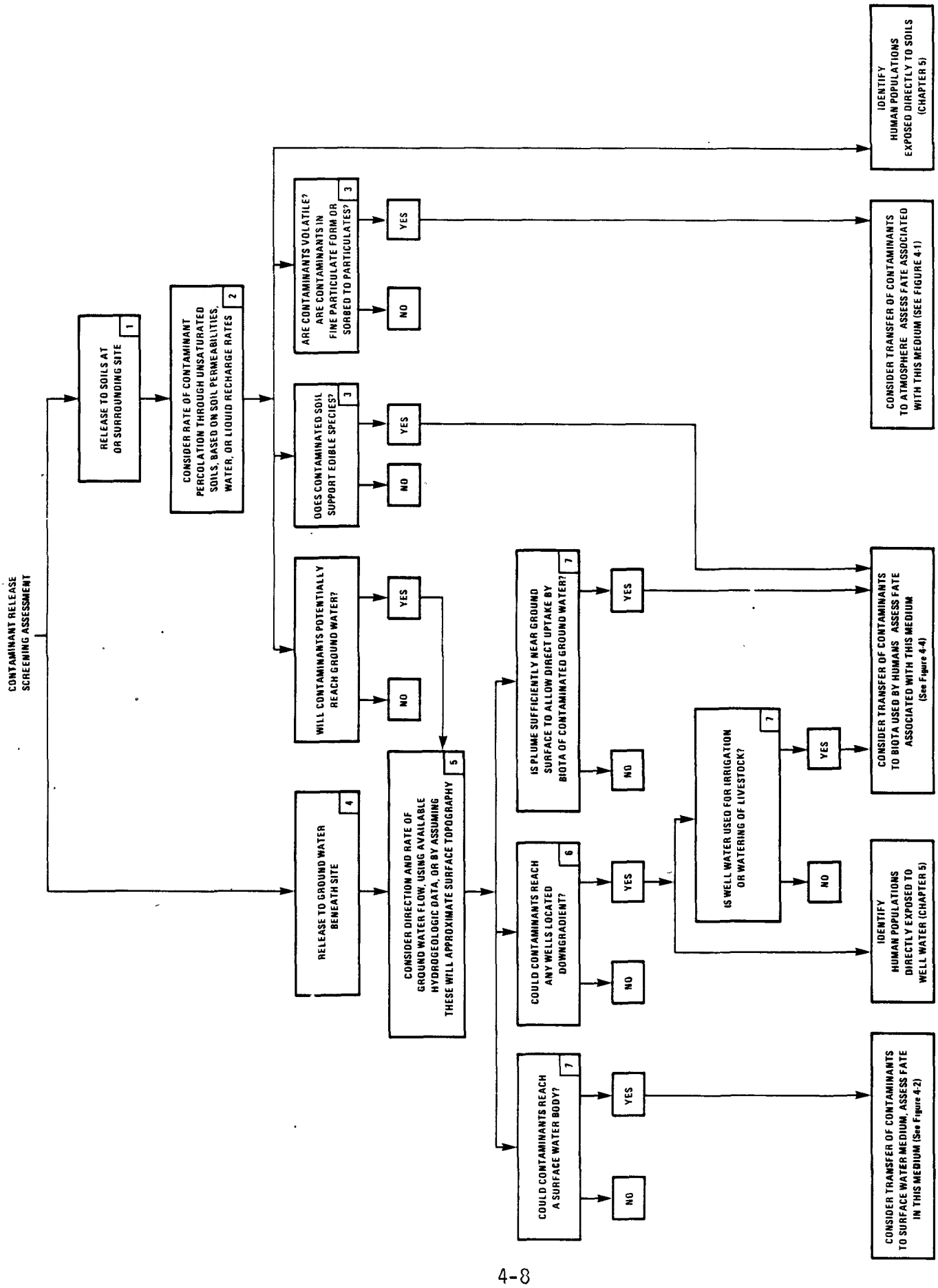

FIGURE 4-3. ENVIRONMENTAL FATE SCREENING ASSESSMENT DECISION NETWORK: SOILS AND GROUND-WATER

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 due to human activities such as irrigation or watering of livestock with well water.

4.2.4 Contaminant Environmental Fate Screening: Biotic Fate

The following numbered paragraphs are provided to facilitate interpretation and application of the biotic fate decision network presented as Figure 4-4. Each paragraph refers to a particular numbered box in the figure.

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 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 biomagnification through the food chain, natural animal migration, or human commercial activity. Food chain biomagnification can result in high concentrations of contaminants in the tissue of edible species not

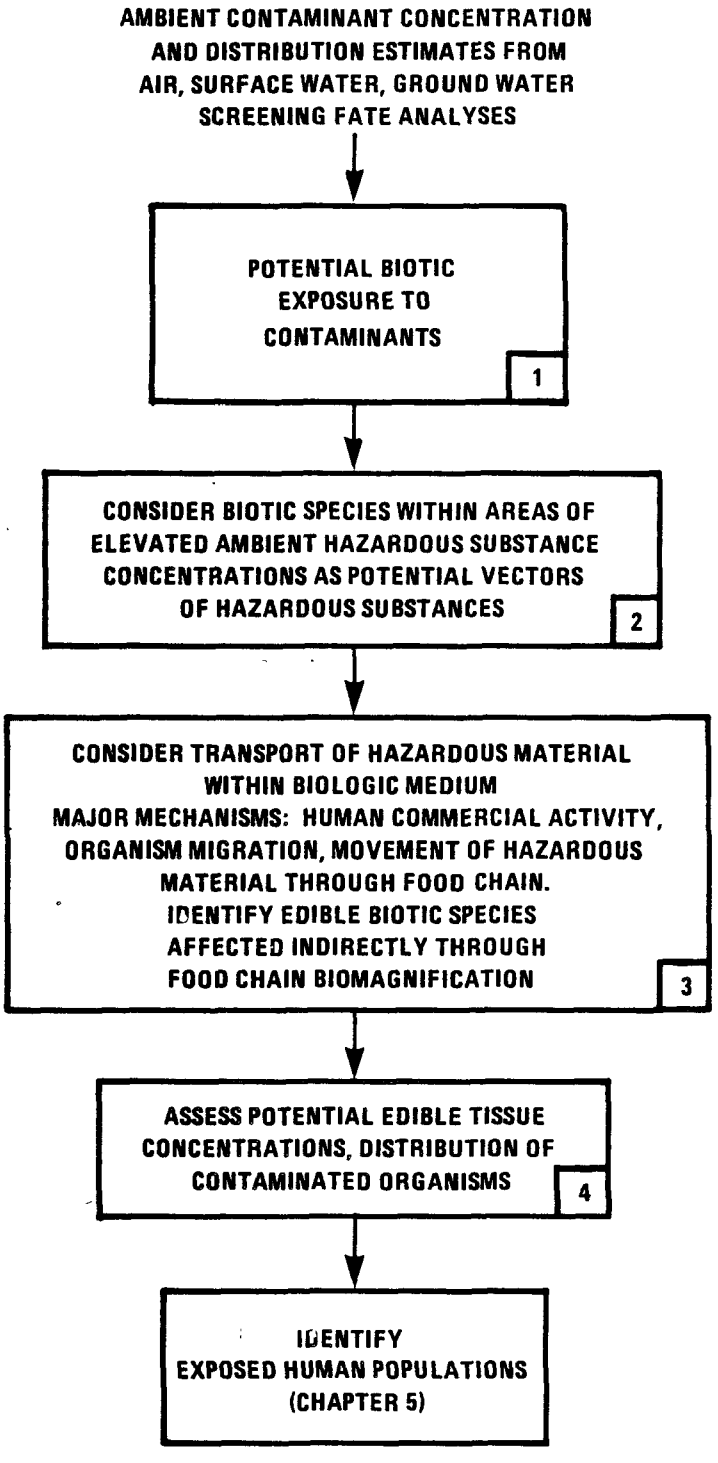

FIGURE 4-4. ENVIRONMENTAL FATE SCREENING ASSESSMENT DECISION NETWORK: FOOD CHAIN

in direct contact with contaminated air, water, or ground water. Human commercial transport and natural migratory behavior of contaminated species can result in 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.

4.3 Quantitative Environmental Fate Analysis

The following subsections provide two forms of guidance for quantitative environmental fate analyses. For each environmental medium, simplified algorithms for calculating important environmental fate terms (contaminant distribution and/or ambient concentrations) are first presented. The discussion of these algorithms is followed by annotated lists of in-depth environmental fate analysis methods and models.

Simplified environmental fate estimation procedures are based on the predominant mechanisms of transport within each medium, and they generally disregard transfer or transformation processes. They produce conservative estimates (i.e., reasonable upper bounds) for final ambient concentrations and the extent of hazardous substance migration. Because the estimates obtained by these procedures serve as input to subsequent identification of exposed populations and exposure estimations, it is important to avoid underestimating or overlooking significant pathways that impact human health. Wherever the simplifying assumptions incorporated into these estimation procedures could lead to underestimation of ambient concentrations or movement of hazardous substances in the environment, this is indicated in the discussion. In general, it will be necessary to use more sophisticated, in-depth analysis techniques (i.e., modeling/monitoring) in such cases.

When more in-depth analysis of environmental fate is required than can be performed with simplified algorithms, the analyst must select the modeling procedure that is most appropriate to the circumstances under study. In general, the more sophisticated models are more data-, time-, and resource-intensive. Models that produce results of greater sophistication than is required for public health evaluation or is supported by the reliability or availability of data should be avoided.

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.

- Form and content of model output. Does it address important questions regarding human exposure, environmental effects? Does it provide all data required as input to further analysis?

As an aid in identifying the important fate processes affecting the substance in question or operative at the site, 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 the provided estimation procedures. By comparing the list of important processes identified for the site with the tabular summary of model features presented at the end of each section, a selection of the model best suited to the requirements of the site can be made.

An excellent guide to the selection of computer-based contaminant fate models can be found in Modeling Remedial Actions at Uncontrolled Hazardous Waste Sites (USEPA 1985e). This document goes beyond providing detailed guidance on the matching of site parameters, data availability, and data needs with model capabilities. It also provides guidance on matching models to remedial alternatives being considered at a site.

Models listed in the following subsections cover a wide range in complexity, capabilities, and resource requirements. The degree of sophistication varies from the simplified algorithms to the highly complex and detailed.

One particular set of computer models is highlighted in the following sections because of its easy accessibility and use, and because of its ability to produce sophisticated analyses of environmental fate. This is the Graphical Exposure Modeling System (GEMS), prepared by the EPA's Exposure Evaluation Division (EED), Office of Toxic Substances (OTS).

GEMS consists of models capable of assessing contaminant fate in air, surface water, ground water, and soil. These fate models are integrated with pertinent data files (containing nationwide soil, land use, and meteorological data, in addition to data on many major river systems, lakes, and reservoirs), user-input data manipulation and storage capabilities, statistical processing programs, and graphics capabilities including 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 for activation of 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, whereupon 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
- 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).*

4.3.1 Atmospheric Fate

(1) Simplified Procedures. The atmospheric fate of substances released from uncontrolled hazardous waste sites can be estimated based on the two predominant mechanisms affecting the movement of airborne substances, advection and dispersion.

The following equation takes these two mechanisms into account and estimates ground-level atmospheric concentrations of pollutants at selected points directly downwind from a ground-level source (Turner 1970):

$$C(x) = \frac{Q}{\pi \sigma_y \sigma_z \mu} \qquad (4\text{-}1)$$

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

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 = 3.141593.

The appropriate dispersion coefficients can be taken from Figures 4-5 and 4-6. 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 very stable (see Pasquill 1961).

Values for wind speed, wind direction, and stability class can be taken from Table 4-1 for estimating maximum ambient concentrations. These values are only recommended if site-specific meteorological data cannot be obtained for the site region; however, the use of site-specific data is highly recommended. The values in Table 4-1 represent reasonable worst-case assumptions for conditions likely to occur at a site for the time periods specified and will therefore result in conservative estimates of ambient concentrations. When using these values, multiply the concentration value obtained from Equation 4-1 by the appropriate percent value in the final column of Table 4-1 to incorporate reasonable worst-case assumptions regarding wind directional variability.

For estimation of long-term mean atmospheric concentrations, a wind speed of 3 meters/second, stability Class D, and the assumption that the wind blows towards the exposure point 30 percent of the time can be used where necessary in lieu of site-specific data, or for very rough conservative estimates.

More accurate estimates of long-term mean atmospheric concentrations can be obtained through use of 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 receptor by applying a weighted average, based on the relative frequency of each stability class and of wind flow toward selected exposure points. Equation 4-2 provides a rough weighted average estimate:

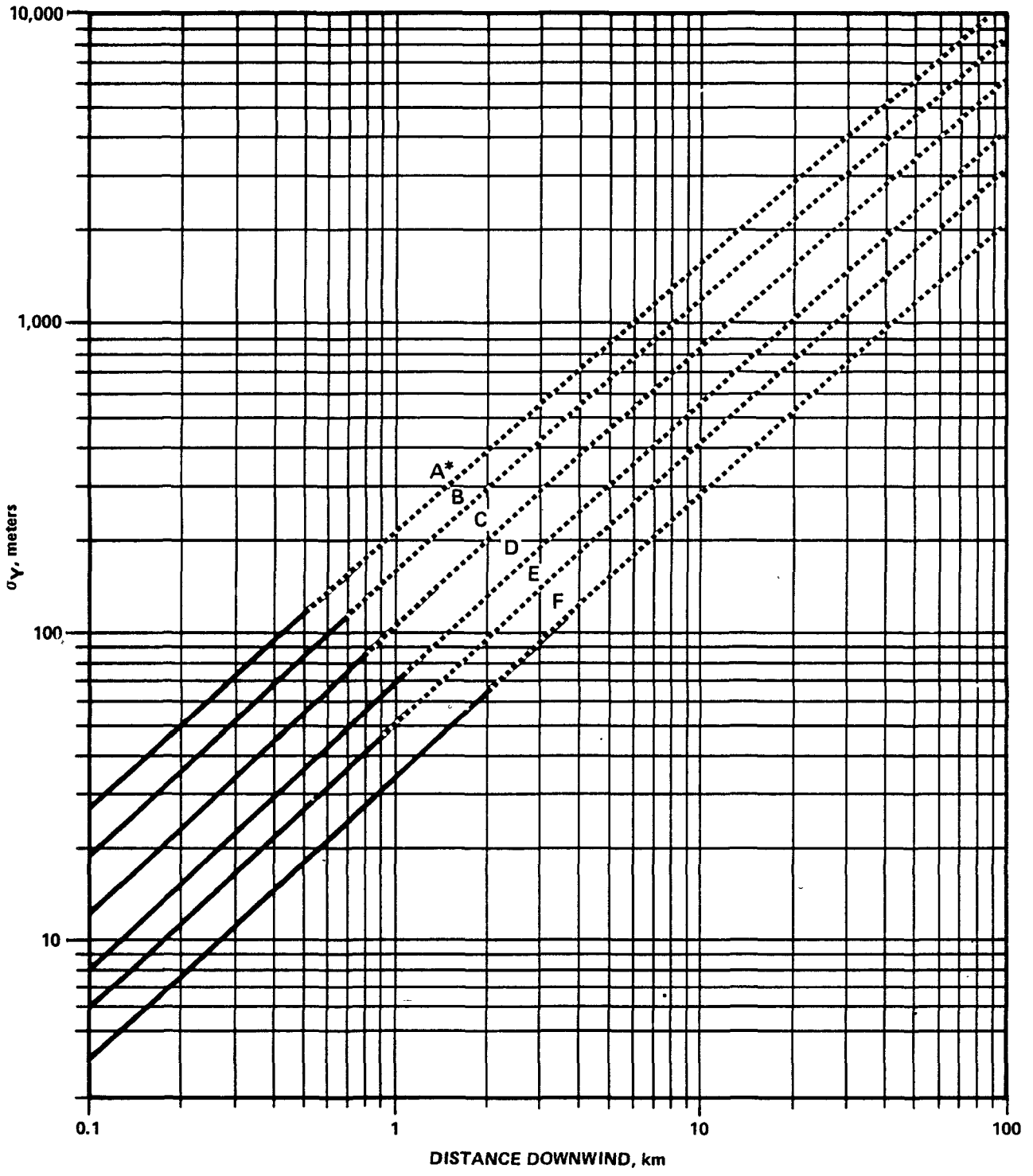

FIGURE 4-5. HORIZONTAL DISPERSION COEFFICIENT AS A FUNCTION OF DOWNWIND DISTANCE FROM THE SOURCE (From Turner, 1970)

* LINES DESIGNATED A THROUGH F REPRESENT DISPERSION COEFFICIENT FUNCTIONS FOR ATMOSPHERIC STABILITY CLASSES A THROUGH F. SEE TEXT FOR SOURCES OF ATMOSPHERIC STABILITY DATA.

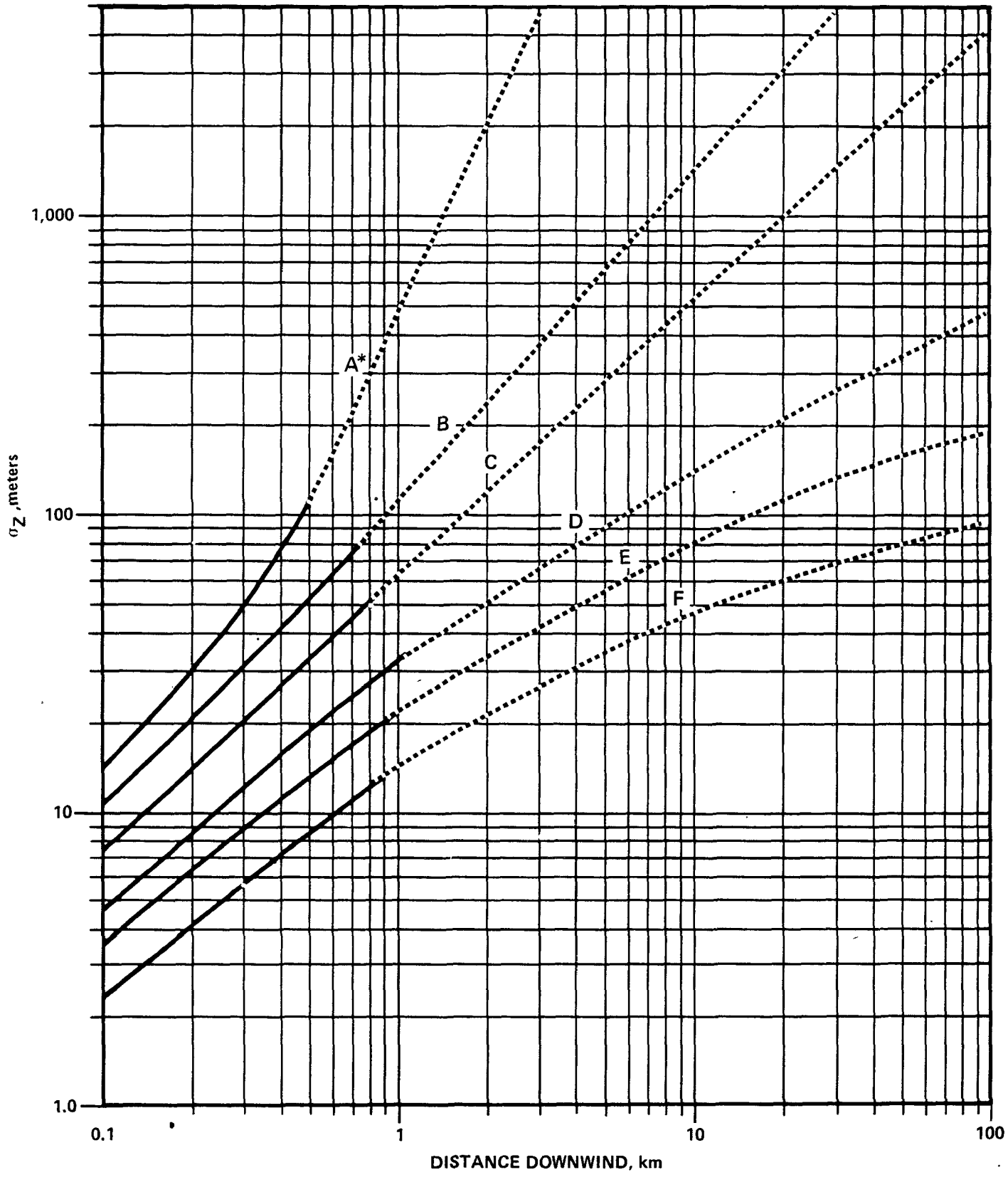

FIGURE 4-6. VERTICAL DISPERSION COEFFICIENT AS A FUNCTION OF DOWNWIND DISTANCE FROM THE SOURCE (From Turner, 1970)

*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 4-1. Assumptions for Calculation of Short-term Maximum Concentrations in Air*

Duration	Wind speed	Stability class	Percent towards exposure point
1 hour	1 m/sec	F	100
24 hour	2 m/sec	E	50
7 days	3 m/sec	D	30

* These assumptions are provided for general guidance only. For some sites, such as deep valleys, these input assumptions may be inappropriate and detailed site-specific data may be required.

$C_A(x)$ = concentration at point x during stability class A (from Equation 4-1).
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 m/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 for all U.S. locations from the National Climate Center (NCC), Asheville, North Carolina (phone: (704) 259-0205).

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 4-3:

$$y_{(x)} = \left(2\ln \bullet \frac{C(X)}{C(CL)}\right)^{1/2} \left(\sigma_y\right) \qquad (4\text{-}3)$$

where

C(CL) = predetermined critical concentration 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 4-1).
σ_y = lateral dispersion coefficient, (length units).

Vary the value for x (downwind distance from the source) input into Equations 4-1 and 4-3, starting at a point near the site* and increasing this value until the value for C(x) (obtained from Equation 4-1) equals the predetermined critical concentration C(CL). Values calculated for y describe the isopleth boundary on either side of the plume centerline.

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

increasing this value until the value for C(x) (obtained from Equation 4-1) equals the predetermined critical concentration C(CL). Values calculated for y describe the isopleth boundary on either side of the plume centerline.

Estimate the area within a plume isopleth using Figure 4-7 (Hilsmeier and Gifford 1962 as presented by Turner 1970), which plots the value $\frac{C(CL)\mu}{Q}$, (relative concentration times wind speed with nomenclature remaining as defined for Equations 4-1 and 4-3) versus isopleth area, for each stability class A through F.

All of the preceding simplified equations provide atmospheric fate estimates based on several simplifying 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 velocity in the downwind direction).

- The substance is conservative (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.

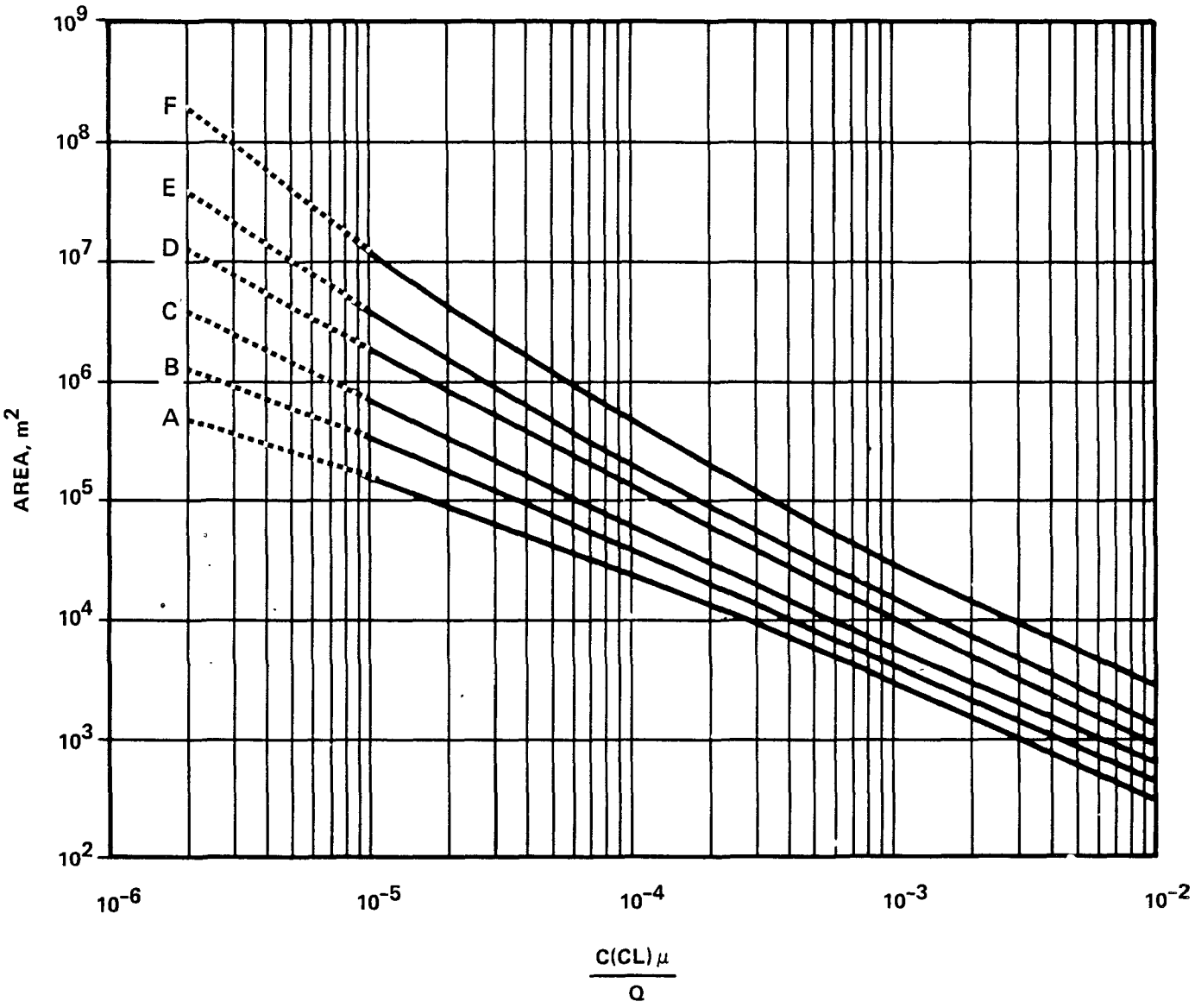

FIGURE 4-7. AREA WITHIN ISOPLETHS FOR A GROUND-LEVEL SOURCE
(Hilsmeir and Gifford 1962, as presented by Turner, 1970)

* CURVES DESIGNATED A THROUGH F REPRESENT FUNCTIONS FOR ATMOSPHERIC STABILITY CLASSES A THROUGH F. SEE TEXT FOR SOURCES OF ATMOSPHERIC STABILITY DATA.

- 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.

- Releases are at ground level, with no initial vertical velocity or heat capable of causing initial plume rise. All vertical transport is a result of dispersion.

(2) In-Depth Analysis. In cases 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. 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.

a. 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.

- 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 due to dissolution/rainout.

- 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.

- Gravitational settling. As stated earlier, this mechanism is most important for particulate hazardous substances, or hazardous substances adsorbed onto suspended particulates, if the particulate matter is more than 20 um 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 (see Hanna and Hosker 1980).

b. 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, it should be noted that 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) also provide rate constants and estimation procedures for these processes.

- 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).

- 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.

- 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) In-Depth Methods and Models. Tables 4-2, 4-3, and 4-4 provide information about computer-based models most appropriate to in-depth analysis of the atmospheric fate of substances released from CERCLA sites. Table 4-2 contains resource requirements, references, and sources for each model; Table 4-3 summarizes their features and capabilities; and Table 4-4 discusses the data requirements of each. Through comparison of the information in these tables with identified site features, site data availability, final output requirements, and resource availability, a selection of the most applicable and cost-effective model can be made.

The Atmospheric Transport Model (ATM) is the most sophisticated of the atmospheric fate models presently integrated into the GEMS system. A detailed description of ATM is provided below. Three other models directly accessible through GEMS (ISC, PTDIS, and PTMAX) are described in Tables 4-2, 4-3, and 4-4.

The ATM (Cylkowski and Patterson 1976) 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 ATM 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 Chapter 5, Exposed Populations). The graphic capabilities of the GEMS package can be used to display ambient concentration as a function of distance or direction from the release site, in the form of bar charts, scatter plots, or circle diagrams. Ground-level plume isopleths can also be depicted in map form (GSC 1982; personal communication with Mr. Loren Hall, EPA-EED).

The following information must be provided by the user of the ATM model (GSC 1982):

Table 4-2. Resource Requirements and Information Sources: Atmospheric Fate Models

Model	Description	Resource requirements	References, sources of document, software
PTMAX	• Steady-state Gaussian plume model • Point source • Short-term • Assumes conservative pollutant • Produces maximum hourly concentrations for each stability and wind speed location of maximum concentration	• Available through GEMS (see Section 4.1) • FORTRAN IV Program, applicable to wide range of computers; has been implemented on UNIVAC 1110 • Approximately 12 K bytes memory required • Software available as part of UNAMAP package for $420	References: Turner and Busse 1973 General Software Corporation 1982 Software: Computer Products, National Technical Information Service (NTIS), Springfield, VA 22161
PTDIS	• Steady-state Gaussian plume model • Point source • Accommodates limit to upward vertical mixing • Short-term • Assumes conservative pollutant • Produces estimates of hourly concentrations at a user-selected downwind distance	• Available through GEMS (see Section 4.1) • FORTRAN IV Program, applicable to wide range of computers; has been implemented on UNIVAC 1110 • Approximately 12 K bytes memory required • Software available as part of UNAMAP package for $420	References: Turner and Busse 1973, General Software Corporation 1982 Software: Computer Products, NTIS, Springfield, VA 22161
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 2500 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

Table 4-2. (continued)

Model	Description	Resource requirements	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 2500 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 • 17K bytes memory required • Technical background in meteorology, air pollution useful	Documentation: Texas Air Control Board 1980
Climatological Dispersion Model (CDM)	• Long-term seasonal or annual • Point or area sources • Gaussian plume model • Simulates non-conservative 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 • 22K bytes storage required • Software available as part of UNAMAP package for $420	Documentation: Busse and Zimmerman 1976 Software: Computer Products, NTIS, Springfield, VA 22161
VALLEY	• Short- or long-term • Simulates plume impact in complex terrain • Provides screening estimates of worst-case short-term concentrations • Provides annual average concentrations • 112-receptor grid • Accommodates nonconservative pollutants • Requires stability array data for long-term option • Requires user-input worst-case meteorological data for short-term screening option	• 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 • Software available as part of UNAMAP series for $420	Reference: Burt 1977 Software: Computer Products, NTIS, Springfield, VA 22161

Table 4-2. (continued)

Model	Description	Resource requirements	References, sources of documentation, software
Industrial Source Complex	• Long-term or short-term point, area, or line sources, single or multiple sources • Models gravitational settling of particulates, providing deposition • Release rates can be varied as a function of time • Not applicable to complex terrain • May provide overly conservative short-term maximum values for calm wind conditions	• Integrated into GEMS • Requires stability array data • Extensive input data required to make use of sophisticated features • FORTRAN IV program language, has been implemented on UNIVAC 140 • Approximately 65 K bytes storage required	Documentation: Bowers et al. 1979 Software: Computer Products, NTIS, Springfield, VA 22161
ATM	• See text, Section 4.2.2	• Integrated into GEMS system, (see Section 4.1) • Program can be executed on IBM, CDC, or VAX computers	Documentation: Patterson et al. 1982 Contact for access to GEMS system: Mr. Loren Hall Exposure Evaluation Division, USEPA Washington, D.C. (202) 382-3931

Sources: Bonazountas 1982; USEPA 1982a; USEPA 1979a.

TABLE 4-3. FEATURES OF ATMOSPHERIC FATE MODELS

	PTMAX	PTDIS	TEM	TCM	COM	VALLEY	ISC	ATM
OUTPUT IN FORM OF CONCENTRATIONS AT RECEPTOR POINTS	●	●	●	●	●			●
OUTPUT IN FORM OF ISOPLETHS OR DATA SUFFICIENT FOR ISOPLETH CHARTING			●	●	●			●
PRODUCES RATE OF DEPOSITION FOOTPRINTS (FOR PARTICULATE RELEASES)							●	●
PRODUCES ANNUAL AVERAGE CONCENTRATION DATA			●	●	●	●	●	●
PRODUCES 24-HOUR MAXIMUM AMBIENT CONCENTRATION DATA	●	●	●			●	●	●
ACCEPTS TIME-VARIANT RELEASE TERMS							●	
HANDLES ROUGH TERRAIN/URBAN SIMULATION				●				●
ACCOUNTS FOR ADSORPTION/SETTLEOUT					●	●	●	●
ACCOUNTS FOR DISSOLUTION/RAINOUT					●	●		●
ACCOUNTS FOR DEGRADATION			●	●	●	●		●
ACCOUNTS FOR VERTICAL DISPERSION	●	●	●		●	●		
ACCOUNTS FOR HORIZONTAL DISPERSION	●	●	●	●	●	●		
MODELS LONGITUDINAL TRANSPORT (ONE-DIMENSIONAL)	●	●		●	●	●		●
MULTIPLE SOURCE						●		●
AREA SOURCE			●	●	●	●	●	●
POINT SOURCE	●	●	●	●	●	●	●	●
HANDLES VOLATILIZATION RELEASES	●	●	●	●	●	●	●	●
HANDLES PARTICULATE RELEASES							●	●

SOURCES: Bonazountas 1982, USEPA 1982a, USEPA 1979a.

TABLE 4-4. DATA REQUIREMENTS FOR ATMOSPHERIC MODELS

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

Sources: Bonazountas 1982; USEPA 1979a; USEPA 1982a.

- Source location (latitude/longitude coordinates or zip code)
- Cover type surrounding the site (on a scale of 1 for grassland to 10 for dense forest)
- Source strength or emission rate, in grams per second
- Emission state (gaseous or particulate)
- If particulate emission, particle size and density
- Molecular weight of pollutant
- Atmospheric half-life of pollutant (calculated on the basis of loss rates due to transfer or transformation processes)

The ATM 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 (monthly, seasonal, annual average) concentration estimates can be developed, and gravitational settling, dissolution/rainout, and intramedia transformation losses can be simulated based on user-input half-life data (GSC 1982).

ATM can be executed on 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 4.3 for access instructions.)

(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 4-1 and 4-3. 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 4-1. When using site-specific data, the most stable atmospheric conditions, lowest wind speed, and greatest percent of wind flow towards the receptor should be used as input to Equation 4-1, along with maximum release rate estimates for the duration of interest. Usually, the receptor nearest the point or area of a ground-level release experiences the highest short-term exposure.

As indicated in Table 4-2, 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.

4.3.2 Surface Water Fate Analysis

The environmental fate of hazardous materials entering surface water bodies is highly dependent on the type of water body. The three major classifications are rivers and streams, impoundments, and estuaries. Methods for estimating contaminant concentrations in the first category are provided below. Because of the diversity in reservoir and estuary types, and the relative complexity of the methods necessary for predicting hazardous material fate in these various environments, approaches that conservatively estimate ambient hazardous material concentrations are beyond the scope of this work. Refer to Mills et al. (1982) for estimation methods covering impoundment and estuary fate assessment.

(1) Simplified Procedures. 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 water body, after dilution of the substance by the receiving water body:

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

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).

In cases where hazardous waste is introduced into a stream through intermedia transfer from air, soil, ground water, or from a 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:

$$C = \frac{T_r}{Q_t} \qquad (4\text{-}5)$$

where

T_r = intermedia transfer rate (mass/time).
Q_t = stream flow rate (volume/time).

Assumptions implicit in these equations are:

- Mixing of the hazardous substance in the water is instantaneous and complete.
- The hazardous material is conservative (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 of substance introduction. 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):

$$MZ = \frac{0.4\ w^2 u}{0.6d\ \sqrt{gds}} \qquad (4\text{-}6)$$

where

MZ = mixing zone length (length units).
w = width of water body (length units).
u = stream velocity (length/time).
d = stream depth (length units).
s = slope of the stream channel (length/length).
g = acceleration due to gravity (32 ft/sec^2).

In addition, 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 4-4 and 4-5.

If the hazardous substance is introduced into a flowing water body 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 above dilution equations (4-4, 4-5) 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 due to 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 using an overall decay coefficient, which represents a combination of all decay and loss rates affecting the removal of a substance from a water body. 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:

$$W(x) = W(0)e^{-K\frac{x}{u}} \qquad (4\text{-}7)$$

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 4-7, and solving this equation for x, as follows:

$$x = -\frac{u}{K}\left(\frac{\ln [W(CL)]}{\ln [W(0)]}\right) \qquad (4\text{-}8)$$

Nomenclature for both equations is as follows:

W(CL) = predetermined critical concentration level (mass/volume).
W(x) = concentration at downstream distance x (mass/volume).
W(0) = concentration immediately below point of introduction (from dilution Equations 4-4, 4-5).
e = exponential function.
K = overall decay coefficient $(time)^{-1}$.
u = stream velocity (length/time).
x = distance downstream from point of introduction (length units).

This equation incorporates the following assumptions:

- Complete mixing.
- Steady-state conditions.
- Longitudinal dispersion is negligible; 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, 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 water body must be known. For this information, see the discussion below (Section 4.4.2), 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 (1979), Dawson, English, and Petty (1980), and USCG (1974).

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

(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 for assessing 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.

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

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

- Sedimentation. Hazardous substances released to a surface water body 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) also provide a procedure for estimation of 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.

- 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, non-polar 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.

b. 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 and Mills (1982), Verschueren (1984), and Sax (1984) provide rate constants for these processes for numerous compounds.

- 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.

- Oxidation. This 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.

- Hydrolysis. Hydrolysis refers to the introduction of a hydroxyl group into a compound, usually either as an addition or as a substitution for another group. Hydrolysis of most compounds is highly dependent on the pH of the water body 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.

- Biodegradation. This is the breakdown of substances through the enzymatic action of biota present in the water. Most biodegradation is carried out by microbial biota. It is a function of 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) In-Depth Methods and Models. Tables 4-5, 4-6, and 4-7 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.

The surface water model presently integrated into the EPA GEMS system is EXAMS. This model is comprehensive in the transport and transformation processes that it incorporates and is versatile in its ability to simulate streams, rivers, ponds, and lakes. It cannot estimate fate in estuaries or tidal systems, and it is limited only to the modeling of the fate of organic compounds.

Because of its relative complexity, EXAMS is data intensive. It requires information on climatic, biological, hydrological, and sediment characteristics; physicochemical properties of the substance, such as molecular weight, solubility, partition coefficients, hydrolysis rate constants, biodegradation rates, etc; and release strength and stream flow rate data.

A data set of average or typical values for water body-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, reverine lakes, and reservoirs, and will be integrated with the EXAMS program. These values will therefore be accessible for fate modeling of the water bodies included (General Software Corp. 1982).

Table 4-5. 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 restrictive	Reference: Mills et al. 1982 Documentation: ORD Publications USEPA, Cincinnati, OH 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 using a more sophisticated model • May be used with hand calculator	Reference: HydroQual 1982 Documentation: William Gulledge 2581 M Street, N.W. Washington, DC 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

Table 4-5. (continued)

Model	Description	Resource requirements, comments	References, sources of documentation, software
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, DC 20037 202-887-1183
Exposure Analysis Modeling System (EXAMS)	• 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 Reserch Information USEPA Cincinnati, OH 45268 513-684-7562 Center for Water Quality Modeling Environmental Research Laboratory USEPA Athens, GA 30613 404-546-3585

Table 4-5. (continued)

Model	Description	Resource requirements, comments	References, sources of documentation, software
Metals Exposure Analysis Modeling System (MEXAMS)	• Steady-state, 3-dimensional compartmental model • Complex computer program • A combination of two models (MINTEQ and EXAMS) 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 • Interactive format • Contains data base with thermodynamic properties of 7 metals	Further information: Yasuo Onishi Battelle Pacific Northwest Laboratories Richland, WA 99352 509-376-8302 Documentation: Center for Water Quality Modeling, Environmental Research Laboratories, USEPA, Athens, GA 30613
Toxic Organic Substance Transport and Bioaccumulation Model (TOXIC)	• Quasi-dynamic, 3-dimensional compartment model • Program language is FORTRAN • Complex biological uptake mechanisms • Models pesticides and in reservoirs and aquatic impoundments • Only time-varying functions for loading, not flows • Good for biological accumulation but lacking in chemical fate mechanisms	• Applicable to IBM 370 and 750 Prime systems • FORTRAN program in batch mode • User support is limited; no user manual is available	Reference: Schnoor et al. 1981 Software: Jerry Schnoor Civil and Environmental Engineering Energy Engineering Division University of Iowa Iowa City, IA 52248 319-353-7262
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. 1980 Software: Center for Water Quality Modeling Environmental Research Laboratory USEPA Athens, GA 30613 404-546-3585

Table 4-5. (continued)

Model	Description	Resource requirements, comments	References, sources of documentation, software
Transient One-Dimensional Degradation and Migration Model (TODAM)	• Time-varying, 1-dimensional model • Second-order decay mechanisms • Models river and estuarine systems • Exterior hydrodynamic model (e.g., EXPLORE) is required 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, for estimation of 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 hydro-dynamic 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 large	References: Onishi 1981 Further Information: Yasuo Onishi Battelle Pacific Northwest Laboratories Richland, WA 99352 509-376-8302

Table 4-5. (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	References: 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 Env. Research Lab Center for Water Quality Modeling Athens, GA 30613 404-546-3546
Estuary and Stream Quality Model (WASTOX)	• 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 32 K bytes storage • Requires 150-300 man hours for setup	Documentation and Software: Dr. John Connolly Environmental Engineering and Science Manhatten College Bronx, NY 10471 212-920-0276 or: Dr. Parmely H. Prichard Environmental Research Laboratory Gulf Breeze, FL 32561 904-932-5311
Chemical and Stream Quality Model (TOXIWASP)	• Time-varying, 3-dimensional model • Comprehensive second-order decay kinetics for organic pollutants • Models rivers and estuaries, can be applied to lakes	• Very data-intensive model • Applicable to IBM 370 or PDP 11/70 • Software in Fortran IV; requires 64 K byte memory • Requires 150-300 man hours for setup	Documentation and Software: Robert Ambrose Center for Water Quality Modeling USEPA Athens, GA 30613 404-546-3546

Source: Versar 1983.

TABLE 4-6. FEATURES OF SURFACE WATER FATE MODELS

	WQAM	SLSA	MICHRIV	CTAP	EXAMS	MEXAMS	TOXIC	HSPF	TODAM	CHNTRN	FETRA	SERATRA	WASTOX	TOXIWASP
PREDICTS PERSISTENCE OF CONTAMINANT FOLLOWING TERMINATION OF RELEASE		●			●	●	●	●	●	●	●	●	●	●
PREDICTS SHORT-TERM MAXIMUM CONCENTRATIONS AT RECEPTORS		●					●	●	●	●	●	●	●	●
PREDICTS LONG-TERM AVERAGE AMBIENT CONCENTRATIONS AT RECEPTORS	●	●		●	●	●	●	●	●	●	●	●	●	●
PREDICTS BIOCONCENTRATION LEVELS OF CONTAMINANTS							●							
PREDICTS METAL SPECIATION						●				●				
PREDICTS CONTAMINANT CONCENTRATION AS A FUNCTION OF DISTANCE FROM SOURCE	●	●	●	●	●	●			●	●	●	●	●	
PARTICULATE POLLUTANTS	●		●	●	●	●			●	●	●	●		
METALS/INORGANICS	●	●	●	●		●		●	●		●	●		
ORGANIC POLLUTANTS	●	●	●	●	●		●	●	●	●	●	●	●	●
NONPOINT SOURCE	●				●	●	●	●	●	●	●	●	●	●
POINT SOURCE	●	●	●	●	●	●			●	●	●	●	●	●
STEADY STATE	●	●	●	●	●	●								
HANDLES DYNAMIC WATER FLOW								●	●	●	●	●	●	●
HANDLES VARYING RELEASE RATES		●					●	●	●	●	●	●	●	●
ACCOUNTS FOR STRATIFICATION	●			●	●	●				●		●	●	●
ACCOUNTS FOR PHYSICAL REMOVAL	●	●	●	●	●	●	●	●	●	●	●	●	●	●
ACCOUNTS FOR DEGRADATION	●	●	●	●	●		●	●	●	●	●	●	●	●
ACCOUNTS FOR DISPERSION				●	●	●	●		●	●	●	●	●	●
MULTIDIMENSIONAL				●	●	●	●				●	●	●	●
1-DIMENSIONAL	●	●	●					●	●	●	●		●	●
ESTUARIES/TIDAL	●			●					●	●	●		●	●
IMPOUNDMENTS	●	●		●	●	●	●	●		●	●	●	●	●
STREAM/RIVERS	●	●	●	●	●	●		●	●	●	●	●	●	●

Sources: Versar; Delos et al. 1984

TABLE 4-7. 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 SIZE OR CONTENT PARAMETERS	OVERALL AQUATIC HALF LIFE VALUES	DISPERSION COEFFICIENTS	SUBSTANCE PHYSICAL/CHEMICAL PROPERTIES	CHEMICAL PARTITION COEFFICIENTS	WATER COLUMN DEGRADATION COEFFICIENTS	BED SEDIMENT DEGRADATION COEFFICIENTS	AVERAGE RELEASE RATES	DYNAMIC RELEASE PATTERNS
WQAM	●	●	●						●				●		●	●			●
SLSA	●	●								●	●					●	●	●	●
MICHRIV	●															●	●	●	●
CTAP	●	●								●	●	●		●		●	●	●	●
EXAMS	●	●		●	●	●	●			●	●	●	●	●	●	●	●	●	●
MEXAMS	●	●		●	●	●	●			●	●	●		●	●	●			●
TOXIC	●	●			●	●	●			●		●	●	●		●	●		
HSPF	●	●	●	●		●						●			●	●	●		
TODAM	●	●								●		●		●	●	●	●	●	
CHNTRN	●	●		●	●	●	●			●		●	●	●	●	●	●	●	
FETRA	●	●								●		●		●		●	●	●	
SERATRA	●	●								●		●		●		●	●	●	
WASTOX	●	●			●	●	●			●	●	●	●	●	●	●	●	●	
TOXIWASP	●	●		●	●	●	●	●				●		●	●	●	●	●	

Source: Vesar 1983a; Delo et al. 1984

(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 4-6 indicates several aquatic fate models capable of estimating both short- or long-term ambient water concentrations that are appropriate to in-depth analysis of the aquatic fate of contaminants released from Superfund sites.

4.3.3 Ground-Water Fate Analysis

(1) Simplified Procedures. The fate of hazardous substances in the soil (unsaturated zone) and in the ground water (saturated zone) after release to these media from an uncontrolled hazardous waste site is determined by many, mainly site specific factors. The two estimation procedures provided below for pollutant transport in these zones incorporate simplifying assumptions for hazardous substance properties as well as the hydrogeology underlying the site. It must be emphasized, however, that certain soil, geological, and hydrological features render these assumptions nonconservative and the presented algorithms inapplicable. These features, highlighted in the discussion of assumptions implicit in these equations, are described in further detail in Subsection 4.3.3(2) below.

The following procedures provide estimates of the rate of contaminant travel and approximate boundaries of the contaminant plume as a function of time elapsed since release. These procedures assume that, after release from a site, contaminants travel vertically downward through the unsaturated zone, dissolve into the ground water underlying the site, and then travel with the advective flow of this ground water. They further assume that contaminants are completely soluble in water and travel at the velocity of leachate or ground water in the unsaturated and saturated zones, respectively.

a. Unsaturated Zone. The following equation is used to estimate the mean rate of downward travel of a hazardous material spread on or just beneath the surface of soils (or deposited by wind, or by water erosion/deposition). It provides the velocity of interstitial pore water downward through the unsaturated zone, and therefore gives the assumed velocity of hazardous substance movement through this zone. This velocity is given by the following algorithm (Enfield et al. 1982):

$$V_{pw} = \frac{q}{\theta} \qquad (4\text{-}9)$$

where

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

Records of estimated percolation rates for the site locality and 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. Department of Agriculture offices.

An estimation procedure can be used for evaluating 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 are available. In addition to the above two sources, 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 following equation provides an estimate of the term q:

$$q = HL + P_r - ET - Qr \qquad (4\text{-}10)$$

where

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

The term HL, representing hydraulic loading from manmade sources, is not significant or quantifiable at many sites. This term is generally only used for sites at which liquids were applied to the site surface (e.g., land application sites), and the volumes and general time periods of application are on record. For such sites, HL is calculated by dividing the volumes of liquid applied by the area of application, and dividing the resultant depth value by the time periods during which the liquid was applied. This HL value is added to other terms in Equation 4-10 only for those time increments during which the liquid application took place. For time increments during which no known or quantifiable liquid application took place, and at sites where HL cannot be quantified at all, the value for HL is zero.

Note that the term HL and Equation 4-10 are not applicable to sites where high-volume releases resulted in saturated conditions or where ponding are known to have occurred.

The average precipitation rate per unit time (Pr) 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:

$$ET = EVAP \times C_{et} \times C_{veg} \qquad (4\text{-}11)$$

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 4-8, which requires climatological and pan descriptive information.

The term C_{veg} is available mainly for agricultural crops (see Table 4-9), 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 is unavailable, a conservative default value for this term is the smallest reasonable value, or 0.6.

Qr, or the average runoff over the study period, is estimated by the method presented in Section 3.5 of this manual, or through other appropriate methods (e.g., Donigian et al. 1983). A more reliable value for this term may 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 Qr = 0, where site-specific data are unavailable or cannot be estimated.

The second independent variable in Equation 4-9, the volumetric water content of the site soil (θ) may be quantified during site investigation through soil sampling and gravimetric analysis. The value for θ obtained in this manner, however, may reflect conditions only at the time of the site investigation, and may not provide a value for θ that is appropriate for the entire period of study.

Table 4-8. Suggested Value for C_{et} Relating Evaporation from a US Class A Pan to Evapotranspiration from 8-15-cm Tall, Well-watered Grass Turf

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

Table 4-9. 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 volumetric water content in the unsaturated zone for the five period of concern may be estimated using the following equation adapted from Clapp and Hornberger (1978):

$$\theta = \left(\theta_s\right) \left(\frac{q}{K_s}\right)^{\frac{1}{2b+3}} \qquad (4\text{-}12)$$

where

- θ = volumetric water content in unsaturated zone (volume/volume or unitless).
- θ_s = volumetric water content of soil under saturated conditions (volume/volume, or unitless).
- q = percolation rate (calculated by Equation 4-10; assumed to be equal to the unsaturated hydraulic conductivity term in the original Clapp and Hornberger equation; depth per unit time).
- K_s = saturated hydraulic conductivity (depth per unit time).
- b = soil-specific exponentical parameter (unitless).

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 4-10, 4-11, 4-12, and 4-13, provide guides for the rough estimation of θ_s, K_s, and the term $\frac{1}{2b+3}$. Representative values from two different sources are presented for K_s (Tables 4-11 and 4-12) and θ_s (Tables 4-10 and 4-13), 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 4-12 equals or exceeds θ_s, it must be assumed that saturated conditions exist. In such cases, use θ_s as the upper bound for the value θ in Equation 4-9.

Similarly, the minimum value for θ that is applicable to Equation 4-9 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 for the study site are those measured empirically during site investigation (if this parameter was evaluated). Where empirical values are not available,

Table 4-10. 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	(1.64)	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.

Table 4-11. 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 4-12. 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}
Fractored igneous and metamorphic rock	10^{-6}	—	10^{-2}
Permeable basalt	10^{-5}	—	1
Karst limestone	10^{-4}	—	1

Adapted from Freeze and Cherry, 1979.

Table 4-13. Representative Values for Saturated Moisture Contents and Field Capacities of Various Soil Types

	Number of Soils	Saturated Moisture Content (θ_s)[a] Mean	± 1 standard deviation	Field capacity (cm^3/cm^3)[b] 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 loan	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.

default values may be taken from Table 4-13. Wherever Equation 4-12 results in a value for θ which is less than the specific retention of the soil, it should be assumed that no downward movement of moisture (and dissolved contaminants) occurred for the associated time increment, and V_{pw} was equal to zero.

Note also that the percolation rate (i.e., the term 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 4-12 $\geq \theta_s$) for the duration of the study period, it must be assumed that saturated conditions exist and that saturated flow prevails. Equation 4-13 in the following subsection provides a means of estimating saturated flow velocities.

Assumptions implicit in equations 4-9 and 4-10 include the following:

- Dispersion and capillary flow in all directions are negligible in relation to the downward velocity of pore water and dissolved contaminants due to gravity.
- Contaminants present at the site dissolve into infiltrating water, without significantly changing the viscosity of the water.
- Contaminants are conservative; degradation and soil adsorption effects are negligible.
- Soils underlying the site are homogeneous and isotropic; macropores resulting in rapid flow do not exist at the site.
- The effects of surface or pore water freezing are negligible.
- The site is located in a region of net precipitation (i.e., HL + Pr > ET) for the majority of time increments considered
- The introduction of water from manmade sources is intermittent and in low-volume increments, rather than as high-volume spill events. These equations are not applicable to situations involving significant ponding of liquids at the site or the establishment of saturated soil conditions.

A more detailed discussion of some of these assumptions and their implications is provided below in section 4.3.3(2).

The mean-estimated velocity value, V_{pw}, when multiplied by the time period of concern during a Superfund investigation, provides a conservative estimate of the depth to which contaminants from the site

have penetrated or will penetrate. This depth estimate should be compared with data for the depth to the underlying aquifer. Where such a comparison suggests that contaminants may have reached or will reach the aquifer, the following saturated zone calculation procedures (Subsection 4.3.3(1)(b), below) should be followed in order to estimate contaminant plume dimensions within the aquifer.

In cases where this procedure indicates the possibility of human exposure to contaminants via ground water, estimates of contaminant concentration in ground water at potential exposure points will be required. Such estimates require as input the rate of contaminant flux through the unsaturated zone and introduction to the aquifer. A rough estimate of the likely upper bounds of contaminant flux to ground water can be developed by multiplying the percolation rate, q, with the area of soil surface contamination, resulting in a volume per unit time influx of moisture. If the soil moisture content is assumed to remain constant, this same volume per unit time represents the water flux from the unsaturated zone to the aquifer. The upper bound for contaminant concentration in this water flux is the solubility of the contaminants in water (assuming no chelating compounds or dissolution agents are present). Thus, contaminant flux to ground water roughly equals contaminant solubility in water multiplied by the volumetric water flux through the unsaturated zone.

Estimates developed by this method must be regarded as preliminary and of low reliability. For an additional, more reliable method of estimating contaminant flux through the unsaturated zone to ground water, the analyst is referred to the estimation procedure presented by Donigian et al. (1983).

b. Saturated Zone. In cases where contaminants are contained in a lagoon or pond, soils below the site are saturated, the unsaturated zone is insignificant or nonexistent, or when the results of the foregoing unsaturated zone fate estimation procedures indicate that contaminants have penetrated the unsaturated zone and reached the ground water, the rate of contaminant migration in the saturated zone is estimated. It is assumed for the purpose of the following estimation that the hazardous contaminants are dissolved into the pond liquid or ground water and travel at the rate of ground-water flow, or as a saturated flow.

For many sites, the ground-water flow rate may have been determined empirically during site investigations. Where measurement data are unavailable, the rate of ground-water or saturated flow can be estimated by Darcy's Law, as summarized by the following equation:

$$V_{pw} = \frac{K_s i}{N_e} \qquad (4\text{-}13)$$

where

V_{pw} = average linear pore water velocity of ground water and contaminant (distance/time).
K_s = saturated hydraulic conductivity of the soil (distance/time).
i = hydraulic gradient (distance/distance).
N_e = effective porosity of the soil (%).

Again, each of the input parameters for Equation 4-13 may have been evaluated empirically during site investigation. If this is not the case, rough estimates for saturated hydraulic conductivity can be taken from the mean values for this parameter presented in Table 4-11, or median values of ranges shown in Table 4-12, based on the general soil or rock type underlying the site. The range values presented in these two tables provide an indication of the uncertainty of using assumed values rather than site data.

Preferably, 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. Alternatively, values for this parameter may be available through several sources including hydrogeological reports from the U.S. Geological Survey, state or local agencies, or nearby university geology or hydrogeology departments. Water levels in existing nearby wells can also provide an indication of hydraulic gradient. Table 4-10 provides values for saturated moisture content, (which is roughly equal to the effective porosity, or N_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. Use of estimated values can be expected to yield very rough approximation of the velocity of contaminant movement through the unsaturated and saturated zones, and the incorporation of a wide margin for error is necessary in order to ensure the desired conservative results.

Equations 4-9 and 4-13, in combination with the time elapsed since release, provide a means of determining whether hazardous substances have potentially reached the ground water underlying the site, and if so, whether they have traveled with ground-water flow to predetermined receptor sites. They also permit estimation of the likelihood of hazardous substances reaching a receptor point within a time frame of future remedial alternative planning. They incorporate many conservative

assumptions (enumerated in the discussion of ground-water fate mechanisms in Section (2) below) regarding contaminant properties and migration, and as such provide worst-case estimates.

The use of these procedures for predicting the effect of remedial actions on ground water contamination is highly dependent on the assessment of the situation before remedial action and the type of remedial action under evaluation. Where preliminary determinations indicate that contaminants have not reached the ground water, remedial actions that eliminate or reduce percolation at the site can be expected to arrest or greatly retard contaminant movement. The effect of this type of remedial action may be estimated through modification of the percolation term (q) in Equation 4-9. If it is determined, however, that hazardous substances have reached ground water, the reduction of percolation or leachate release to ground water will usually result in a plug-type flow of the contaminant plume already in the ground water before the remedial action began. This plug of contaminated water will usually continue to migrate downgradient at the rate determined by Equation 4-13.

If, through the application of these estimation procedures, it is determined that the contaminant will reach receptor sites either as a plume or plug flow, ground-water concentrations of hazardous substances must be estimated at the affected receptor sites.

To provide useful estimates, quantitative procedures for ground-water contaminant concentrations must account for several complex fate mechanisms and therefore require lengthly calculations (see for example the procedure presented by Wilson and Miller 1978) beyond the scope of this manual. The analyst is referred to two documents for simplified approaches to these estimation procedures. The first is the article by Kelly (1982) which presents a code for the Texas Instruments model 58 or 59 programmable calculators. This code performs the calculations required for the estimation procedure presented by Wilson and Miller (1978) and greatly reduces the time required for ground-water concentration estimation. The second document is that by Donigian et al. (1983) which presents the same basic estimation procedure in nomographic form, eliminating the need for lengthy calculations.

(2) <u>In-depth Analysis</u>. The assumptions that form the basis of Equations 4-9 and 4-13, and the estimation procedures for ground-water concentration presented by Donigian et al. (1983) and Kelly (1982) limit the application and reliability of these methods. These assumptions are detailed below. The analyst should especially be able to identify situations where ground-water concentrations may be greater than those predicted by the estimation procedures, or where estimation of contaminant flow and ground-water concentrations indicate that the concentration of hazardous substances in ground water may present a hazard to human receptors.

The following is a discussion of the fate mechanisms that must be considered during the planning of an in-depth analysis or the selection of a ground-water fate model. The assumptions and limitations of the foregoing estimation procedures with respect to these fate mechanisms are also discussed.

(a) Dispersion. This process is brought about by velocity variations in individual pore spaces and by diffusion of hazardous substances over a concentration gradient. Dispersion causes the "spreading" of a contaminant plume as it moves farther from a point of release, and occurs in three dimensions unless a barrier prevents this process in one or more directions (see Aquitards, below). While dispersion affects the rate of movement of a plume boundary, this effect is disregarded by Equations 4-9 and 4-12. The estimates of one-dimensional flow obtained by these equations is nevertheless valid for the development of conservative or worst-case estimates of contaminant migration. The estimation procedures presented by Kelly and Donigian et al. do take into account dispersion in the estimation of contaminant concentrations in ground water.

(b) Hydrogeologic Characteristics Affecting Fate. The following hydrogeologic characteristics determine the rate and direction of contaminant transport. The assumptions concerning these characteristics incorporated into the foregoing estimation procedures are stated in each case.

- Permeability. The above estimation procedures assume isotropy and homogeneity of the subsurface medium through which the leachate or ground water travels. Isotrophy refers to a uniform hydraulic conductivity irrespective of the direction of water movement (e.g., horizontal conductivity is equal to vertical conductivity). Homogeneity refers to uniform hydraulic conductivity characteristics at all points within the soil (i.e., no impermeable layers or strata with different conductivity characteristics). In actuality, this is rarely the case; most soils are heterogeneous and anisotrophic (Kufs et al. 1983). Permeability of a soil can vary widely from one area to another or with depth. Often, soil grain size fluctuates gradually with depth or unpredictably in multilayered media (Kufs et al. 1983). If such variation exists and can be reliably quantified, average permeability values can be used as input to provide estimates of ground-water fate. Computer models with routines accounting for various levels of permeability can be used for more accurate predictions.

- Aquitards. Aquitards are zones of relative impermeability, which act as barriers to movement of ground water. Aquitards can be above, on either side of, or below an aquifer, confining its shape and therefore the movement of contaminants. The estimation

procedures provided above assume that contaminants move vertically through the unsaturated soil zone and horizontally in the ground water. As such, these procedures do not account for directional flow diversions caused by aquitards, and the effects of such diversions are often difficult to model even with computer-based procedures. The foregoing estimation procedures do assume, however, that there is an aquitard below the aquifer, which limits mixing and transport downward (Donigian et al. 1983, Wilson and Miller 1978). Absence of such an aquitard, resulting in unlimited dispersion downward, therefore, renders these procedures unreliable, as they may overestimate ground-water concentrations of hazardous substances at shallow wells, and underestimate those at deep withdrawal points. A more sophisticated model accounting for this feature should be used in such situations.

Fissures in an aquitard further complicate prediction of plume migration, unless these leaky aquitards can be described reliably (Kufs et al. 1983). When such features are known to exist, but cannot be accurately described or quantified, only the monitoring of ground water can provide accurate information regarding hazardous material concentrations at exposure points.

- Solution cavities, fractures. The rock material that underlies, confines, or is itself a medium of ground-water flow in many cases contains irregular fractures, or cavities, formed by dissolution of the rock material by water. Ground-water flow rate through these fissures can be extremely rapid compared to that in surrounding material (Kufs et al. 1983). Because of irregularity in size, shape, and direction of fissures, attempts to model ground-water flow in areas exhibiting these features are unreliable. Contaminated liquids can flow through fractures and cavities largely unimpeded and undiluted by retardation or dispersion processes. When these conditions exist, the only reliable method of determining concentrations at wells or springs is monitoring. Predictions as to whether a particular point in the aquifer may be affected by plume migration can often only be made through tracer studies.

- Hydrologic fluctuations. Percolation and hydrologic head gradients, and therefore ground-water flow rates and directions, can fluctuate significantly with seasonal or long-term fluctuation in precipitation, snow melt, evapotranspiration, surface runoff, and flooding (Kufs et al. 1983). The estimation procedures provided assume a constant or average flow rate, and a consistent or average direction of flow. For conservative estimates of ground-water contaminant concentrations whenever wide hydrologic fluctuation occurs, use low flow rates as inputs to the ground-water concentration estimation procedures of Donigian et al. (1983) or Kelly (1982).

c. Transfer and Transformation Processes. The following are the most significant processes that remove hazardous substances from ground water through transfer to other media, or through degradation of the substance. The Darcy's Law estimation procedure disregards these processes, and thereby provides worst-case estimates of ground-water contaminant migration. If such worst-case estimates indicate potential human hazard and estimation of contaminant concentration in ground water is required, the concentration estimation procedures of Kelly (1982) and Donigian et al. (1983) do allow the incorporation of an overall decay coefficient.

The coefficient represents the combined removal action of all of the processes that are active at a site and for the contaminant in question. It is developed through summation of the individual decay rates of each process. Appropriate individual decay rates or overall decay coefficients have been developed for numerous substances, and are available in the technical literature. Sources for such data include: Callahan et al. (1979); Dawson, English, and Petty (1980); Mabey et al. (1982); Sax (1979); U.S.C.G. (1974); and Verschueren (1984). Methods of estimating decay coefficients are presented by Lyman et al. (1982).

- Volatilization. This mechanism can be important if the hazardous substance in question has a high vapor pressure or is insoluble and less dense than water. If the aquifer has a large surface area near the soil surface, or if the unsaturated soil layer is especially porous or thin, volatilization rates can also be enhanced. Transport rates of the hazardous substance in the gaseous phase through the unsaturated soil zone and through the air away from the soil-air interface are important determinants of the rate of volatilization.

- Hydrolysis. This is a pH-dependent process for most substances. Hydrolysis rates are chemical specific and dependent on the presence of available hydroxyl or hydronium ions in the ground-water medium.

- Biodegradation. Enzymatic action of biota present in the unsaturated soil and ground water results in the biodegradation of some hazardous substances. Biodegradation is a function of the population and metabolic characteristics and rates of the biotic agents in question.

(d) Retardation. The rate of movement of hazardous substances through the aquifer is usually not the same as that of the ground water itself, because of the action of the following mechanisms of retardation. These mechanisms are not accounted for by Equation 4-9 or

the Darcy's Law equation. The procedures presented by Donigian et al. (1983) and Kelly (1982) account for sorption, but not for the effects of viscosity, filtration or entrapment. Results of these estimation procedures, then, are rendered less reliable in situations where these latter three retardation factors exist, and may predict ground-water concentrations significantly lower than actual levels. Use in-depth analysis techniques or models that incorporate these factors whenever they may be important.

- Filtration. Hazardous substances in suspended particulate form, or that are converted to suspended solid form from solution as the result of precipitation or flocculation, can be filtered out of the ground-water medium. The rate of filtration depends on the relationship between average soil pore size and average size of the suspended particulate hazardous substance. Because precipitation and flocculation are reversible processes that are dependent on the concentration of the hazardous substance in ground water, filtration tends to slow but not arrest movement of most hazardous substances within this medium.

- Sorption. This term encompasses several processes by which substances in ground water or the unsaturated soil zone are attached to soil particles. Sorption rates are a function of the ionic exchange capacity, the organic carbon content of the soil, and properties of the hazardous substance. Soil/water partition coefficients have been developed for many contaminants of importance (see Callahan et al. 1979, and Mabey et al. 1982), and estimation procedures are provided by Delos et al. (1984), Donigian et al. (1983), and Lyman et al. (1982). Sorption is also a reversible process and tends, therefore, to retard rather than stop hazardous substance migration within ground water.

- Entrapment. Because of minor eddies in ground water, portions of hazardous substances dissolved or suspended can disperse into and become temporarily trapped in dead-end pores or fractures in the medium. This process occurs at a rate that is a function of the porosity and interconnectedness of pore spaces in the soil medium.

- Viscosity. High concentrations of hazardous substances dissolved in ground water can significantly raise the viscosity of the solution. Hazardous substances released into the medium in liquid form are often significantly more viscous than water. The effective permeability of soil decreases with increasing viscosity of the solution passing through it, and viscous solutions are therefore transported through the subsurface soil medium at a slower rate than that predicted for water or dilute solutions of

contaminant. This results in more gradual downward movement of the contaminant through the unsaturated zone, plume boundaries closer to the site than predicted by Equations 4-9 and 4-13, and higher concentrations within the plume than predicted by the method presented by Donigian et al.

e. Immiscible contaminants and multi-phase flow. All of the foregoing estimation procedures incorporate the assumption that the contaminants under study dissolve almost entirely in ground water, and that their movement can be approximated through minor modification of or direct comparison to ground-water flow. However, the contaminant compounds likely to be encountered at Superfund sites vary widely in solubility; many are immiscible with water. These compounds, upon release to soils or ground water, tend to migrate as discrete non-aqueous phases (Mackay et al. 1985). Such immiscible compounds that are denser than water are most likely to concentrate at the bottom of an aquifer, just above the underlying aquitard, while compounds less dense than water are most likely to "float" at the uppper surface of the zone of saturation. Non-aqueous phases commonly have distinct migration properties and may flow at different velocities and in different directions than water in both the unsaturated and saturated zones. Velocities of immiscible contaminants through the unsaturated or saturated zones can be several times that of water.

(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 for these useful compilations of in-depth methods: USEPA 1985d; Van Geunchten and Alves 1982, Walton 1984, and Javendel et al. 1984.

Tables 4-14, 4-15, and 4-16 provide information regarding several modeling procedures for the in-depth assessment of the ground-water fate of hazardous substances. Two of the models in Tables 4-14, 4-15, and 4-16 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.

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). The model handles two types of waste pertinent to uncontrolled hazardous waste sites, radioactive and chemical. One of eight source configurations can be selected: a point source; line sources aligned in one of three different ways with respect to ground-water flow; area

Table 4-14. 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 3 layers of soil types, permeabilities	• Integrated into GEMS (see Section 4.1) • 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, DC 202-382-3931
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
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, CA 94303 415-493-1864

Table 4-14. (continued)

Model	Description	Resource requirements, comments	References, sources of documentation, software
Saturated zone			
Random Walk Standard Transport Model (RWSTM)	• 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-1D	• 3-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. 1982

Table 4-14. (continued)

Model	Description	Resource requirements, comments	References, sources of documentation, software
Sandria Waste Isolation Flow and Transport Model (SWIFT)	• 3-dimensional • Transport processes of advection, dispersion simulated • Sorption, degradation processes accounted for • Appropriate for waste-injection, waste-isolation modeling	• 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 • 1984 version to be released late 1984 or 1985	Documentation: Reeves and Cranwell 1981; Finley and Reeves 1978 Software: National Energy Software Center, Argonne National Laboratories, Argonne, IL 60439 Information: Intera Environmental Consultants, Inc. 11999 Katy Freeway, Suite 610 Houston, TX 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 nonographic, 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

Table 4-14. (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 tansport/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, TN 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: Kowihow and Bredehaeft 1974
SESOIL and AT 123D	See foregoing descriptions of individual models.		

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

TABLE 4-15. FEATURES OF UNSATURATED ZONE AND GROUND-WATER FATE MODELS

	SATURATED ZONE	UNSATURATED ZONE	1-DIMENSIONAL	2-DIMENSIONAL	3-DIMENSIONAL	ORGANIC SUBSTANCES	INORGANIC SUBSTANCES	HANDLES TIME-VARIANT HYDROLOGICAL FLOW, METEOROLOGY	ACCOUNTS FOR ADSORPTION/DISPERSION	ACCOUNTS FOR RETARDATION MECHANISMS (ANISOTROPHY AND/OR HETEROGENEITY)	ACCOUNTS FOR PERMEABILITY VARIATION	ACCOUNTS FOR AQUITARD ZONES	ACCOUNTS FOR LEAKY AQUITARDS	ACCOUNTS FOR TRANSFORMATION/DEGRADATION	ACCOUNTS FOR METALS SPECIATION	ACCOUNTS FOR VOLATILIZATION TO GROUND-WATER FROM UNSATURATED ZONE	PROVIDES CONTAMINANT MASS/RATE OF RELEASE	PROVIDES CONTAMINANT PLUME BOUNDARIES OF DISTANCE FROM THE SITE	PROVIDES CONTAMINANT CONCENTRATIONS AS A FUNCTION OF DEPTH FROM THE SURFACE	PROVIDES AVERAGE GROUND-WATER CONCENTRATIONS AT SELECTED POINTS	PROVIDES GROUND-WATER CONCENTRATION PROFILES OVER TIME AT SELECTED POINTS
SESOIL		●	●			●	●	●		●	●				●	●	●	●			●	
PESTAN		●	●			●			●	●	●				●			●			●	
HELP		●	●			●	●	●		●												
RWSTM	●		●	●		●	●	●	●	●	●	●	●		●		●		●	●		●	●
CFEST & UNSAT-1D	●	●		●	●	●	●	●	●			●						●				●	●
SWIFT	●		●	●	●	●	●	●	●	●	●	●		●					●	●	●		●
LPMM	●			●		●	●		●	●		●			●				●	●		●	●
FEMWASTE & FEMWATER	●	●		●		●	●	●	●	●	●	●			●				●	●	●	●	●
STDM	●		●	●		●	●	●	●			●						●	●	●	●	●	●
AT123D	●		●	●	●	●	●		●	●					●		●			●	●	●	●

Sources USEPA 1982, Brown et al. 1983, Kufs et al. 1983, Versar 1983b

TABLE 4-16. DATA REQUIREMENTS FOR UNSATURATED ZONE AND GROUND-WATER FATE MODELS

	SOIL TYPES	SOIL POROSITIES	SOIL PERMEABILITY/HYDRAULIC CONDUCTIVITIES	ORGANIC CARBON CONTENT	SOIL BULK DENSITY	CLAY CONTENT	ION EXCHANGE CAPACITY	AQUIFER THICKNESS/UNSATURATED ZONE DEPTH	AQUIFER ELEVATIONS/HEAD PRESSURES/ HYDRAULIC GRADIENT	MEASURED OR EXTERNELLY CALCULATED GROUND WATER FLOW RATES	EVAPOTRANSPIRATION REGIME	PRECIPITATION REGIME	TEMPERATURE REGIME	SUNLIGHT FLUX	VEGETATIVE COVER	WINDSPEED REGIME	DISPERSION COEFFICIENTS	ARTIFICIAL REMOVAL/RECHARGE TO AQUIFER (E.G. PUMPING)	NATURAL RECHARGE RATES (I.E. DUE TO RAINFALL)	SITE AREA, TERRAIN, SLOPE PARAMETERS	RUNOFF RATES	EXPOSURE POINT COORDINATES OR GRID	RELEASE MECHANISM/PARAMETERS	VARIABLE RELEASE RATES	TIME STEP INCREMENT	SUBSTANCE PHYSICAL/CHEMICAL PROPERTIES	SUBSTANCE DECAY CONSTANTS	PRESENCE OF COMPLEXANS	PARTITION COEFFICIENTS	RETARDATION COEFFICIENTS	BACKGROUND OR INITIAL CONCENTRATIONS	
SESOIL	●	●	●	●		●	●	●			●	●	●	●	●	●			●	●	●		●	●		●	●	●	●	●	●	●
PESTAN		●	●		●			●			●	●			●	●	●		●		●			●		●	●		●	●		
HELP			●	●	●						●	●							●	●	●		●	●		●						
RWSTM		●	●		●			●	●	●		●					●	●	●			●		●	●					●	●
CFEST & UNSAT 1D	●	●	●		●			●	●		●	●	●		●	●	●	●	●		●			●			●	●		●	●
SWIFP		●	●						●	●			●				●	●	●				●	●	●	●				●	●
LPMM		●	●					●	●	●							●		●				●				●			●	
FEMWASTE & FEMWATER		●	●						●	●		●					●		●						●		●			●	
STDM		●	●					●	●								●	●				●			●						●
AT123D		●	●		●			●	●								●	●				●	●	●	●	●	●			●	●

Sources: USEPA 1982, Brown et al 1983, Kuhs et al 1983, Versar 1983b

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 due to 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 4.1 above). It is written in FORTRAN and can be installed on a wide range of computer types.

(3) Short- and Long-term Concentration Calculations. Long-term average ground-water concentrations of contaminants at receptor 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 the methods of Kelly or Donigian et al. through input of time-weighted average values for the above parameters. Several of the in-depth analysis models tabulated in Section 4.5.2 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 receptor points are obtained by examination of the ground-water concentration profile at the selected exposure point over time, and identification of the period of maximum concentration.

4.3.4 Biotic Pathways

(1) Estimation Procedures. An assessment of the fate of hazardous material in biotic populations is conducted after the fate of this material in the air, water, and ground water has been estimated. 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 physicochemical 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:

(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 concentration. This assumption closely represents the behavior of many water-borne contaminants, although recent studies suggest that for many hazardous substance tissue concentration is not very strongly related to water column concentration. 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 about 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, BCF values reported in technical literature can be used. 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, 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 (1980), Veith et al. (1980) for instructions for BCF estimation procedures.

(2) Terrestrial animals. Very few 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 and found that the fat/diet BCF 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 3- to 4-orders of magnitude, however. Hence, this method of tissue concentration estimation must be considered semiquantitative at best.

Human exposure to contaminants via the terrestrial animal pathway can only be reliably determined 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) 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 available. 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 semi-quantitative 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.

5.0 QUANTITATIVE ANALYSIS OF EXPOSED POPULATIONS

5.1 Introduction

The results of contaminant release and fate analyses provide the basis for assessing exposed populations. In this assessment, environmental contamination data are compared with populations data to determine the likelihood of human contact with contaminants of concern. 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. 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 6.

5.2 Exposed Populations Screening

Consistent with the preceding analyses, exposed populations screening is primarily qualitative. This evaluation draws on the results of contaminant fate analysis (presented in Chapter 4) to determine the liklihood and extent of human population contact with contaminants.

Exposed populations screening is guided by the decision network provided in Figure 5-1. The following numbered paragraphs are provided to facilitate interpretation and application of the exposed populations decision network presented as Figure 5-1. Each paragraph refers to a particular numbered box in the figure.

1. Human exposure via inhalation should be evaluated for contaminants that have migrated or may, in the future, migrate from the site into air (either directly or indirectly via intermediate transfer). The assessment should consider contaminated dust as well as volatile compounds. For screening purposes, comparison of contaminant concentration isopleths with maps of the local area will identify the potential for such human population inhalation exposure. However, the user should realize that such exposure can occur in recreational areas as well as in residential, commercial, or industrial areas and therefore should interpret local area maps accordingly.

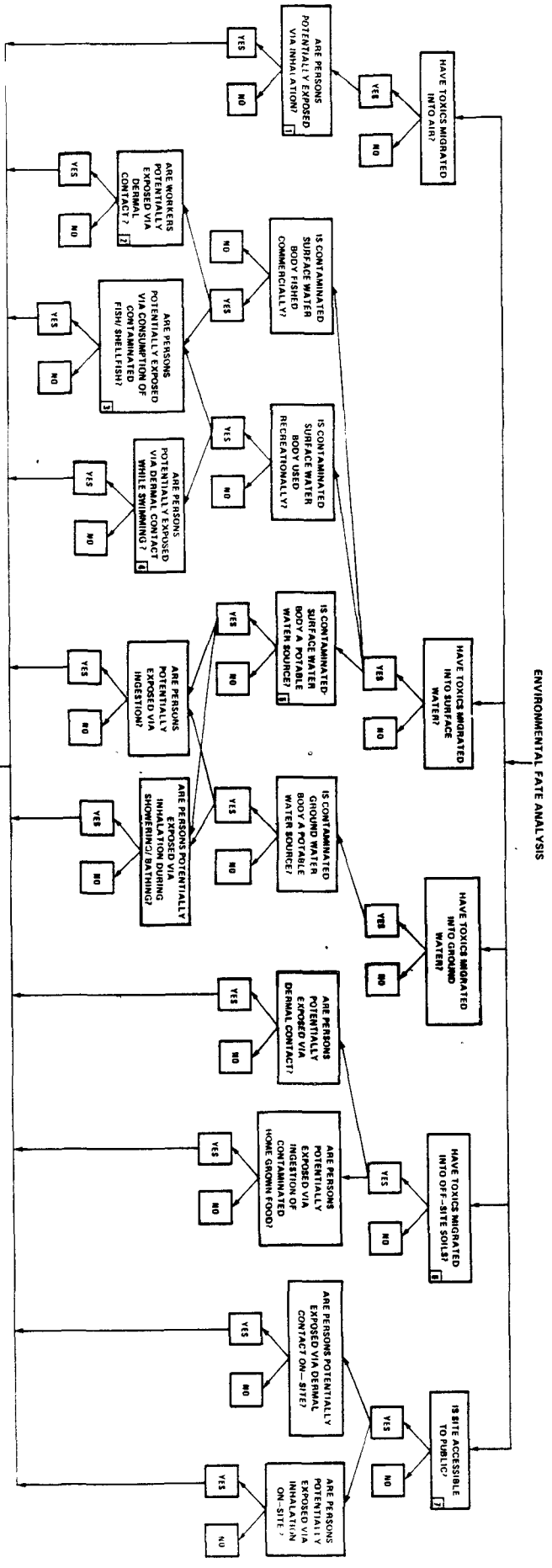

FIGURE 5-1 EXPOSED POPULATIONS DECISION NETWORK

2. In cases where surface water bodies 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 subject waters are commercially fished, the potential for worker exposure, via dermal contact with contaminated water, can also be considered, 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, significant exposure to persons consuming the catch may result. 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. In exposed population screening, the analyst need only determine whether waters identified in the environmental fate analysis as receiving contaminants from the hazardous waste site are used commercially or recreationally.

4. Persons who swim in contaminated waters can experience dermal exposure to toxics over their entire body. Therefore, the existing or potential degree to which the local population uses contaminated water bodies (fresh or marine) for swimming should be evaluated during screening.

5. If contaminated ground or surface waters are used as sources of potable water, the population served may experience considerable drinking water-related ingestion exposure. Similarly, the population may also be exposed to toxics via both dermal absorption and inhalation (for volatiles only) while showering or bathing. For 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. Persons who grow their own fruit or vegetables at home may experience additional exposure from ingestion of food grown in contaminated soils. Again, 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 come in contact with any remaining debris. Such activity may result in inhalation or dermal exposure. For screening purposes, the proximity of residential areas to the site should indicate the potential for direct access by children.

5.3 Quantitative Exposed Populations Analysis

Quantitative analyses of potentially exposed human populations comprises three distinct steps, which are illustrated in Figure 5-2. First, the results of environmental analysis are compared with data identifying and enumerating nearby human populations to bound 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 determining those groups within the exposed population that, because of the specific health effects of some pollutants, would experience a higher risk than 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. High risk groups could include women of childbearing age, the chronically ill, infants/children, and the elderly. While most Superfund studies will consider only the exposed population as a whole and not disaggregate discrete subpopulations, in certain cases such detailed population analysis may be warranted for in-depth studies. For example, if a chemical substance is determined to be teratogenic, enumeration of women of childbearing age may be required.

Age and sex influence the average ventilation 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 the characterization of populations and use of 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?", activity analysis further refines the evaluation by addressing the question "How and to what level are component portions of this population exposed?". This involves determining the exposed population's mix of activities. Comprehensive, highly detailed analysis can encompass the range of indoor, outdoor, and in-car subject population activities. However, for Superfund Feasibility Studies, average values for activity-related considerations usually suffice.

5.4 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.

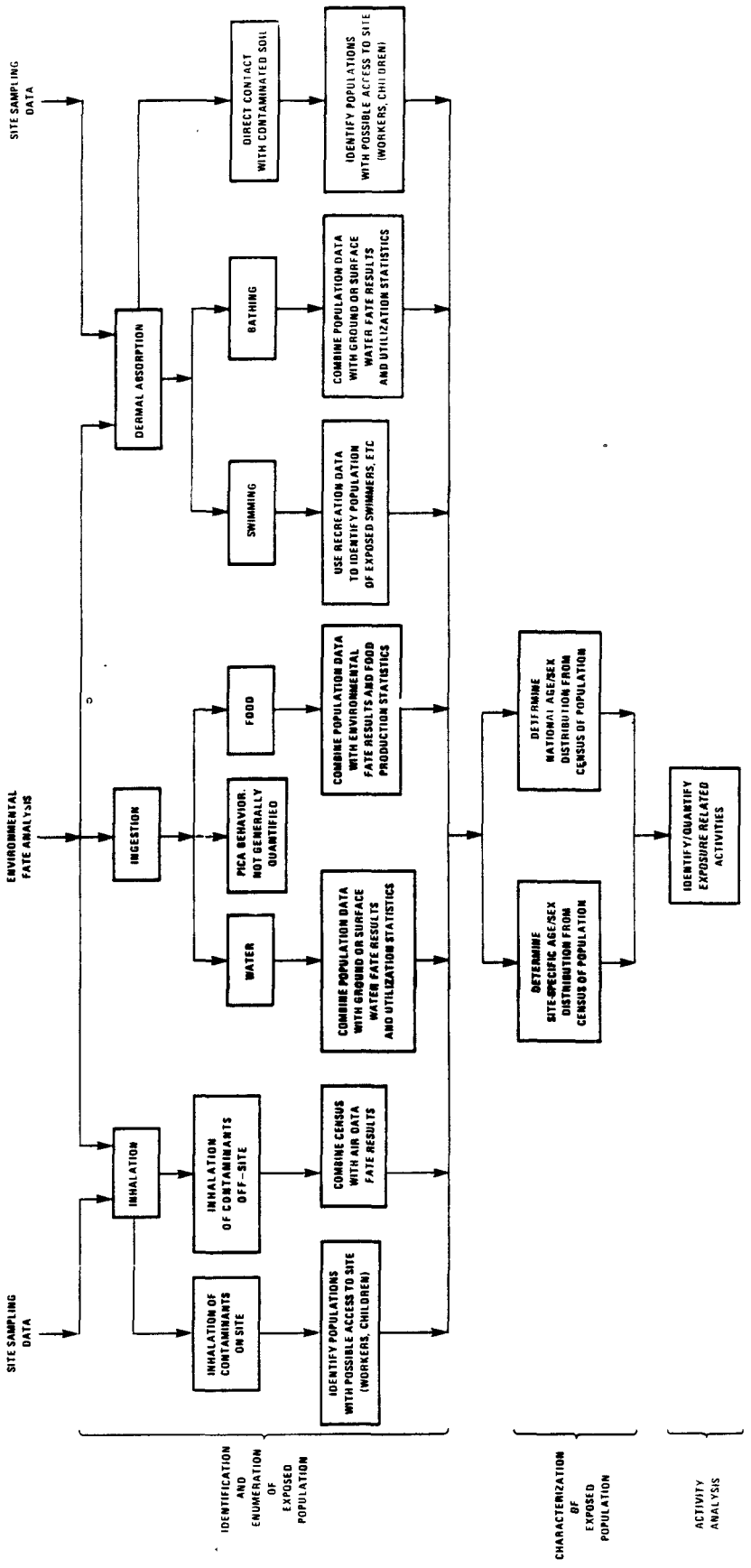

FIGURE 5-2. QUANTITATIVE EXPOSED POPULATION ANALYSIS

The data collected in the Census are organized according to geographic areas, and within these, according to Census-defined statistical areas and government units. Population data, therefore, 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 Standard Metropolitan Statistical Areas (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 5-1.

Table 5-1. Regional Census Bureau Offices

Atlanta, GA	404/881-2274
Boston, MA	617/223-0226
Charlotte, NC	704/371-6144
Chicago, IL	312/353-0980
Dallas, TX	214/767-0625
Denver, CO	303/234-5825
Detroit, MI	313/226-4675
Kansas City, KS	913/236-3731
Los Angeles, CA	213/209-6612
New York, NY	212/264-4730
Philadelphia, PA	215/597-8313
Seattle, WA	206/442-7080

5.4.1 Populations Exposed via Air

An especially 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 via 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. The 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-OTS. Special arrangements can be made for others to use the data. Inquiries should be directed to the Chemical Fate Branch Modeling Team of EPA-OTS in Washington, D.C. A detailed discussion of ATM is presented in Chapter 4 of this manual.

Where sites are accessible, the potential for children entering and exploring or playing on the site should be evaluated. On-site, children may experience inhalation exposure to contaminated dust, volatiles, or both. 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 (1985) reports that in 1983, 50.2 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 (Zoning Board, etc.) may be able to supply information on the liklihood 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.

5.4.2 Populations Exposed via Surface Water or Ground Water

Geographically-defined sources of aquatic, recreational dermal exposure, such as river reaches downstream of an uncontrolled hazardous waste site, can be identified through an examination of Environmental Fate Analysis results. 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, the following national average value from the Bureau of Outdoor Recreation (USDOI 1973) can be used: 34 percent of the total population swims outdoors in natural surface water bodies (including oceans, lakes, creeks, and rivers).

All persons in the service area of 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. Information on public departments or private drinking water treatment companies that use ground water as their raw water supply, and also the number of households drawing water from private wells, will generally be available from these sources.

5.4.3 Populations Exposed via Food

Exposure to contaminated food will usually be associated with fruit and vegetables grown in home gardens, or with game residing in or utilizing 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 identify the total number of households in a given geographic area. Then the data presented in Table 5-2, which provides 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

Table 5-2. U.S. Home Fruit and Vegetable Garden Use, 1977 (USEPA 1980b)

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

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).

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 2.71 persons in the average household (Bureau of the Census 1985), one can estimate the actual exposed population by multiplying 2.71 by the number of licensed hunters or fishermen in the area.

5.4.4 Populations Exposed via 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 via 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. For any site located in the vicinity of residential areas, the degree of access to children should be considered. Bureau of the Census data can be used as described in Section 5.4.1 to estimate the number of local children who may access the site.

In addition, workers conducting activities at the site (other than remediation) may have direct dermal contact with contaminated soils. Section 5.4.1 also provides general guidance for the identification and enumeration of exposed worker populations.

5.5 Population Characterization

After exposed populations have been identified and enumerated, they can be characterized by age and sex factors. The physiological parameters that determine 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. Average values

will generally be used for Superfund studies, but characterization of exposed populations also permits the determination of exposure distributions within the population at large and the delineation of specific high risk subpopulations.

The Census Publication series General Population Characteristics (PC80-1-B) provides 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 provides a series of microfiche containing this information at the Census tract level (only available by SMSAs).

In the case of exposure via 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 1985), to approximate the population distribution in the area of concern.

5.6 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, therefore, experience a higher level of exposure to airborne contaminants.

Activity analysis allows refinement of certain parameters used in the calculation of exposure:

- Inhalation rate
- Frequency of exposure
- 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.

6.0 EXPOSURE CALCULATION AND INTEGRATION

Integrated exposure analysis is conducted for only those contaminants determined to have complete exposure pathways, that is, those contaminants that are released and migrate from the site and that do contact receptor human populations. Therefore, no screening evaluation is included in the exposure integration process. Calculation of exposure incurred is traditionally the final step in the quantitative exposure assessment process. However, it can also be viewed as a component of public health evaluation. Therefore, the material detailed in this chapter is also discussed in the Superfund Public Health Evaluation Manual (USEPA 1985d).

Exposure is defined as the amount of pollutant contacting body boundaries (skin, lungs, or gastrointestinal tract). Exposure calculation considers how often receptors come into contact with contaminants in specific environmental media, the mode of such contact, and the amount of contaminated medium that contacts 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 developed. 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 constitutes an inhalation exposure event). Event-based exposure estimates take into account the concentration of contaminant in the medium via which exposure occurs, the rate of contact with such media (inhalation rate, ingestion rate, etc.), and the duration of each event.

The assessor can convert event-based exposure values to final exposure values by multiplying the exposure per event by the frequency of exposure events over the time frame being considered. Short-term exposure is based on the number of exposure events that occur during the short-term time frame (10 to 90 days), while long-term exposures are based on the number of events that occur within an assumed 70-year lifetime.

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 receptor population. For Superfund studies, an average adult body mass of 70 kg will usually be adequate for this conversion. However, 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 alternate body mass values. Similarly, average values for activity-related parameters (e.g., inhalation rate) generally will suffice for Superfund site evaluations. For special situations and detailed exposure analysis, assessors can refer to the discussion of activity data in Freed et al. (1985).

The following sections address the exposure calculation process specific to each exposure mechanism. Data management sheets designed to facilitate the organization and tabulation of data in the exposure calculation process are presented in Appendix C.

6.1 Inhalation Exposures

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:

$$IEX = D \times I \times C \qquad (6\text{-}1)$$

where

- IEX = estimated inhalation exposure per event (mass of contaminant per event)
- D = duration of an exposure event (hours per event)
- I = average inhalation rate of exposed persons (cubic meters per hour)
- C = contaminant air concentration throughout the exposure period (milligrams per cubic meter of contaminated air).

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). This assumption is not always well-founded, however. 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, however, 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, conservative estimates of exposure can be developed by assuming that all residents spend the entire day within the contaminated zone. In this case, a duration value of 24 hours per day would be used. However, 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 reasonably be 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.

In general application, an average adult value for inhalation rate can be used. 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.

A more precise estimate of inhalation rate can be derived by generating time-weighted average inhalation rates. The basis for this calculation is microenvironment-related data and activity stress levels/ventilation rates associated with the individual microenvironment. If this level of detail is warranted, inhalation rates presented in Table 6-1 can be used. Direction for developing time-weighted average inhalation rates is provided in Freed et al. (1985).

For ambient inhalation exposure calculation, contaminant air concentration values should be obtained from the results of the environmental fate analysis. However, in one case, concentration values will have to be calculated in the exposure integration stage of the exposure assessment. As previously mentioned, 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 turbulance in combination with the elevated temperature of shower water can result in significant release of volatile components.

Various approaches exist for estimating contaminant concentrations indoors, which depend on a number of factors, including the room air volume, air exchange and mixing factors, contaminant concentration

Table 6-1. 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, 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. 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 Methods for Assessing Exposure to Chemical Substances in the Ambient Environment, Volume 2 of Methods for Assessing Exposure to Chemical Substances.

in the water, the amount of water used, and the manner in which a contaminant 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 indoor air contaminant concentration estimation techniques. For both showers and baths, the assessor should assume a continuous contaminant release during the bathing/showering period. Values for the other varible factors mentioned above can be obtained from Versar (1985).

6.2 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:

$$DEX = D \times A \times C \times Flux \qquad (6\text{-}2)$$

where

DEX = estimated dermal exposure per event (mass of contaminant per event
D = duration of an exposure event (hours per event)
A = skin surface area available for contact (cm^2)
C = contaminant concentration in water (weight fraction)
Flux = flux rate of water across skin ($mass/cm^2/hr$).

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.

It is important to note that dermal exposure to contaminants in water presents special problems. Such exposure scenarios involve the body's external surface being brought into contact with an ever-replenished supply of contaminant (i.e., the water in which one swims or bathes is turbulent; thus, contaminants adjacent to the skin are replaced as water containing the full complement of contaminants displaces that from which contaminants have been removed by absorption). For example, to assess dermal exposure to an individual swimming in contaminated waters, one must know what mass of contaminant contacts the body. Since exposure to the entire mass of contaminant in the area of the water body does not occur, exposure must be calculated somewhat differently for the dermal route than for other exposure mechanisms. A simplified approach to this problem assumes 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 flux rate of water across the skin boundary is assumed to be the factor controlling the contaminant absorption rate. According to Scheuplein and Blank (1971) (as reported in USEPA 1979b), the flux rate of water through human skin ranges from 0.2 to 0.5 $mg/cm^2/hr$. It is recommended that, for Superfund Feasibility Study analyses, the higher value be used so as to generate a conservative, worst-case estimate. In this special case, exposure essentially equates with dose; this is unavoidable because of the exposure mechanism involved. In all other exposure cases, contaminant dose is evaluated separately as part of the public health evaluation (see USEPA 1985c).

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
- Duration of exposure = 2.6 hours/day.

Dermal absorption of waterborne contaminants may constitute an exposure route of very significant magnitude. The factors that influence dermal absorption of chemicals are the nature of the compound (molecular weight, lipophilicity), the presence of other compounds that might facilitate passage of a chemical though the skin (e.g., chelating or complexing agents), and 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 significantly in the presence of corrosive agents such as acids or by means of abrasion of the skin (Klaasen 1975). 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 from 29 to 91 percent of the total dose incurred, with the average being approximately 64 percent. The importance of the dermal exposure route is 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.

In situations where persons are likely to become exposed to contaminants in drinking water, the dermal exposure associated with bathing or showering should also be considered. Bathing/showering exposure can be assessed in the same manner as has been discussed for swimming. Generally, an average frequency of one bath or shower per day can be assumed and the duration of each event can be estimated at 20 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 will not be disaggregated by age groups, it is recommended that both availability values be used to represent a general range of exposure for the total swimming or bathing population. Both availability figures cited below are 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 per event as follows:

$$DEX = WF \times A \times DA \qquad (6\text{-}3)$$

where

DEX = dermal exposure (mg/event)
WF = weight fraction of chemical substance in soil (unitless)
AV = skin surface area exposed per event (cm^2/event)
DA = dust adherence (mg/cm^2).

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) provides 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 Substances 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. Therefore, contact frequency should be estimated on a case-by-case basis, based on knowledge of the site and its environs.

6.3 Ingestion Exposure

6.3.1 Food

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, if appropriate.

USDA source materials listed in Section 5.2.3 are also useful in quantifying the amount of contaminated food ingested. The Food Consumptions 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 constitutes an ingestion route of special significance, since certain contaminants of concern tend to biomagnify in the food chain. This phenomenon results in predator fish exhibiting tissue concentrations of contaminants at levels greatly in excess of the ambient concentration in the water body. An

average daily fish ingestion rate for the U.S. population has been estimated as 6.5 grams per day (USEPA 1980c). It has been estimated that persons for whom fish constitutes a major portion of the overall diet 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. 1979) 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.

6.3.2 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 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 1980d) can be used for Superfund site analyses. Frequency of drinking water exposure is daily.

6.4 Exposure Integration

The final step in the exposure assessment process for uncontrolled hazardous waste sites is the integration of all exposures experienced by individual receptor 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, however, that in some cases individual populations may be exposed to a given chemical in a particular medium via more than one exposure scenario. For example, persons who swim in contaminated waters may obtain their drinking water from the same contaminated water body. 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 facilitate organization of the results of exposure calculation and integration.

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APPENDIX A

INDEX TO VARIABLE TERMS

Appendix A. Index to Variable Terms

Term Used	Definition	Units	Equation(s) in which term is used	Source
Chapter 3				
E	Potential annual wind erosion soil loss	(mass/area/time)	3-1	calculated
I'	Soil erodibility index	(dimensionless)	3-1	site data and literature
K'	Soil ridge roughness factor	(dimensionless)	3-1	site data and literature
C'	Climatic factor	(dimensionless)	3-1	literature
L'	Field length along the prevailing wind direction	(feet)	3-1	site data and literature
V	Vegetative cover factor	(dimensionless)	3-1	site data
E_{VT}	Emission factor for vehicular traffic	(kg/vehicle kilometer traveled; lb/vehicle mile traveled)	3-2	calculated
k	Particle size multiplier	(dimensionless)	3-2; 3-3	see text
s	Silt content	(%)	3-2; 3-3	site data, SCS Soils 5 File
S_P	Mean vehicle speed	(kph; mph)	3-2	site data
W	Mean vehicle weight	(Mg; tons)	3-2	site data
w	Mean number of wheels	(dimensionless)	3-2	site data
D_p	Number of days with at least 0.254 mm (0.01 in) of precipitation per year	(dimensionless)	3-2	Figure 3-2
E_{HE}	Emission factor for heavy equipment (batch dump) operations	(kg emission/Mg material moved; lb/ton)	3-3	calculated
U	Mean wind speed	(m/s)	3-3	National Climatological Data Center, Asheville, NC

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
H	Drop height	(m)	3-3	site data
M	Material moisture content	(%)	3-3	site data
Y	Dumping device capacity	(m_3)	3-3	site data
E_i	Emission rate of toxic component i	(g/sec)	3-4; 3-9; 3-10; 3-12; 3-16	calculated
D_i	Diffusion coefficient of component i	(cm^2/sec)	3-4; 3-5; 3-6; 3-13	calculated
A	Contaminated area	(cm^2; areas; ha)	3-4; 3-9; 3-10; 3-12; 3-16; 3-20; 3-23; 3-25; 3-26; 3-27	site data
C_{is}	Saturation vapor concentration of component i	(g/cm^3)	3-4	calculated
P_t	Soil porosity	(dimensionless)	3-4; 3-13	site data; SCS Soils 5 File
d_{sc}	Effective depth of soil cover	(cm)	3-4	site data
M_i	Mole fraction of toxic component i in the waste	(g/g)	3-4	site data
T	Temperature	(°K, °C)	3-5; 3-8; 3-11; 3-14; 3-17; 3-18	site data
MW_i	Molecular weight of contaminant i	(g/mole)	3-5; 3-6; 3-8; 3-10; 3-18	literature
MW_a	Molecular weight of air	(g/mole)	3-5	see text
$\sum V_1$, $\sum V_2$	Molecular diffusion volumes of toxic contaminant (V_1) and air (V_2)		3-5	literature and calculated

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
P_a	Absolute pressure	atm	3-5	site data
D'	Known diffusion coefficient of a compound with molecular weight and molecular diffusion volume close to that of the unknown (D_i)		3-6	see text
MW'	Molecular weight of the selected compound corresponding to D'	(g/mole)	3-6	literature
β	Soil bulk density	(g/cm^3)	3-7; 3-26; 3-27; 3-28; 3-29	site data, SCS Soils 5 File
ρ	Particle density	(g/cm^3)	3-7	see text
p	Vapor pressure of the chemical	(mm Hg)	3-8	literature or estimated (see text)
R	Gas constant	(62.3 mm Hg-liter/k-°mol; 8.2×10^{-5} atm-m^3/-mol-°k)	3-8; 3-14; 3-17	see text
C_i*	Vapor concentration of compound i	(g/cm^3)	3-9; 3-10	site data
V_y	Mean landfill gas velocity in the soil pore spaces	(cm/sec)	3-9	see text
k_{iG}	Gas-phase mass transfer coefficient of chemical i	(cm/s)	3-10; 3-17	calculated
MW_{H_2O}	Molecular weight of water	(g/mole)	3-11	see text
k_iG, H_2O	Gas phase mass transfer coefficient for water vapor at 25°C		3-11; 3-17	calculated

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
C_s	The liquid-phase concentration of component i	(g/cm^3)	3-12; 3-16; 3-20	site data
t	Time measured from sampling time	(seconds)	3-12	site data
d	Depth of dry zone at sampling time	(cm)	3-12; 3-20	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)	3-12; 3-20	calculated
H_i'	Henry's Law constant in concentration form	(dimensionless)	3-13; 3-14	calculated
H_i	Henry's Law constant	($atm\text{-}m^3/mol$)	3-14; 3-17	literature
h	Depth from soil surface to the bottom of the contaminated region	(cm)	3-15	site data
K_i	Overall mass transfer coefficient	(cm/sec)	3-16; 3-17	calculated
k_{iL}	Liquid phase mass transfer coefficient	(cm/sec)	3-17	calculated
Mw_{O_2}	Molecular weight of oxygen	(g/mole)	3-18	see text
k_L,O_2	Liquid phase mass transfer coefficient for oxygen at 25°C		3-18	literature
E_{Ai}	Average release of contaminant i	(mass/time)	3-19; 3-20; 3-30	calculated
V_c	Volume of contaminated region	(cm^3)	3-19	site data

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
C_i	Concentration of contaminant i	(g/cm^3, kg/ha, lb/acre)	3-19; 3-26; 3-27	site data
E	Total release rate of contaminant i obtained by summing all above-listed releases of the contaminant at the site	(g/sec)	3-19	calculated
$Y(S)_E$	Sediment yield in tons per event	(metric tons)	3-21; 3-28	calculated
a	Conversion constant		3-21; 3-22; 3-24; 3-25	see text
V_r	Volume of runoff	(acre-feet, m^3)	3-21; 3-22	calculated
q_p	Peak flow rate	(ft^3/sec, m^3/sec)	3-21; 3-25	calculated
K	The soil-erodibility factor. Obtained from the local Soil Conservation Service office	(commonly expressed in tons per acre per R unit)	3-21	site data, literature
L	The slope-length factor	(dimensionless)	3-21	see Figures 3-3 through 3-5
S	The slope-steepness factor	(dimensionless)	3-21	see Figures 3-3 through 3-5
C	The cover factor	(dimensionless)	3-21	see text and Table 3-5
P	The erosion control practice factor	(dimensionless)	3-21	see text
Q_r	Depth of runoff	(in, cm)	3-22; 3-23; 3-25; 3-29	calculated
R_t	The total storm rainfall	(in, cm)	3-23; 3-25; 3-29	National Climatological Data Center, Asheville, NC; USDC (1961)
S_w	Water retention factor	(in, cm)	3-23; 3-25	calculated
CN	The SCS Runoff Curve Number	(dimensionless)	3-24	Table 3-4

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
T_r	Storm duration	(hour)	3-25	National Climatological Data Center; Asheville, NC; USDC (1961)
S_s	Sorbed substance quantity	(kg, lb)	3-26; 3-28	calculated
D_s	Dissolved substance quantity	(kg, lb)	3-27; 3-29	calculated
θ_c	Available water capacity of the top cm of soil	(dimensionless)	3-26; 3-27	calculated (see text)
K_d	Sorption partition coefficient	(cm^3/g)	3-26; 3-27	literature
PX_i	Sorbed substance loss per event	(kg, lb)	3-28	calculated
PQ_i	Dissolved substance loss per event	(kg, lb)	3-29	calculated
B	Dissolved <u>or</u> sorbed loss per storm event (i.e., PX_i or PQ_i)	(kg, lb)	3-30	calculated (see text)
N	Number of "average" storm events in 70 years	(dimensionless)	3-30	National Climatological Data Center, Asheville, NC; USDC 1961 (see text)
$Y(S)_A$	Annual soil loss in runoff	(tons)	3-31	
R_r	Rainfall and runoff factor	(dimensionless)	3-31	

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
Chapter 4				
x	Distance from site to selected exposure point	(length)	4-1; 4-2; 4-3; 4-7	site data
C(X)	Atmospheric concentration of substance at distance X from the site	(mass/volume)	4-1; 4-3	calculated
Q	Release rate of substance from site to atmosphere	(mass/time)	4-1	calculated
σy	Atmospheric dispersion coefficient in the lateral (crosswind) direction	(length)	4-1; 4-3	Figure 4-1
σz	Atmospheric dispersion coefficient in the vertical direction	(length)	4-1	Figure 4-2
m	Mean wind speed	(length/time)	4-1	site data, Table 4-1
π	The value pi = 3.1416	(dimensionless)	4-1	-------
$\bar{C}(X)$	Average atmospheric concentration of substance at point X over long term	(mass/volume)	4-2	calculated
W(X)	Relative annual frequency of wind flow towards point X	(dimensionless)	4-2	site data
$C_A(X)$	Atmospheric concentration at point X during stability Class A	(mass/volume)	4-2	calculated
f_A	Relative annual frequency of stability Class A for wind flow towards point X	(dimensionless)	4-2	site data
A,B,C, D,E,F	Stability classes (A=unstable, F=stable) according to Pasquil classification system	(dimensionless)	4-1; 4-2	site data, Table 4-1

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
C(CL)	Predetermined critical atmospheric concentration level	(mass/volume)	4-3	air quality criteria
$Y_{(X)}$	perpendicular distance from point X on plume centerline to the C(CL) isopleth boundary	(length)	4-3	calculated
C	Concentration of substance in stream water	(mass/volume)	4-4; 4-5	calculated
C_e	Concentration of substance in effluent	(mass/volume)	4-4	contaminant release analysis
Q_e	Effluent flow rate	(volume/time)	4-4	contaminant release analysis
Q_t	Combined effluent and stream flow rate	(volume/time)	4-4; 4-5	site data
T_r	Intermedia substance transfer rate	(mass/time)	4-5	site data, calculated
MZ	Length of mixing zone downstream of effluent release to stream	(length)	4-6	calculated
W	Width of water body	(length)	4-6	site data
U	Stream velocity	(length/time)	4-6; 4-7; 4-8	site data
d	Stream depth	(length units)	4-6	site data
s	Slope of stream bed	(dimensionless)	4-6	site data
g	Gravitational acceleration constant	(32 ft/sec^2)	4-6	-----
W(X)	Water concentration of substance at downstream distance X	(mass/volume)	4-7; 4-8	calculated
W(CL)	Predetermined critical water concentration level	(mass/volume)	4-8	water quality crieria

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
W(0)	Water concentration of substance immediately below point of introduction to stream	(mass/volume)	4-7; 4-8	calculated
K	Overall aquatic decay coefficient	($time^{-1}$)	4-7; 4-8	literature, estimated
e	Exponential function	-----	4-7	-----
V_{pw}	Interstitial pore-water velocity or ground-water velocity	(length/time)	4-9; 4-13	calculated
q	Average percolation or recharge rate	(depth/time)	4-9; 4-10; 4-12	site data, calculated
θ	Volumetric water content of soil	(dimensionless)	4-9; 4-12	site data, calculated
HL	Hydraulic loading from manmade sources	(depth/time)	4-10	site data, calculated
Pr	Precipitation rate	(depth/time)	4-10	site data
ET	Evapotranspiration rate	(depth/time)	4-10; 4-11	site data, calculated
Q_r	Runoff rate	(depth/time)	4-10	site data, calculated
EVAP	Evaporation rate	(depth/time)	4-11	site data
C_{et}	Correction factor for converting pan evaporation rate to evapotranspiration rate for turf grass	(dimensionless)	4-11	Table 4-8
C_{veg}	Correction factor for converting turf grass evapotranspiration to that for other vegetative cover	(dimensionless)	4-11	Table 4-9, see text
θ_s	Saturated volumetric soil-water content	(dimensionless)	4-12	site data, Table 4-10

Appendix A. (continued)

Term Used	Definition	Units	Equation(s) in which term is used	Source
b	Soil specific exponential function	(dimensionless)	4-12	Table 4-10
K_s	Soil hydraulic conductivity	(length/time)	4-12; 4-13	site data, Table 4-11
i	Hydraulic gradient	(dimensionless)	4-13	site data
N_e	Soil effective porosity	(%)	4-13	site data, Table 4-12

APPENDIX B

Suggested Outline for Exposure Assessment

Suggested Outline for Exposure Assessment Section of the Remedial Investigation Report

1. Summary

   1.1 Purpose and scope
   1.2 Significant release mechanisms
   1.3 Impact on potential receptors
   1.4 Organization of the report

2. Contaminant Release Analysis

   2.1 Site contaminants
      - Contaminants present at the site
      - Contaminants selected for analysis (from health assessment report)
   2.2 On-site sources of hazardous substance release
   2.3 Estimation of substance-specific release rates
      - Short-term
      - Long-term

3. Exposure Pathways and Environmental Fate

   3.1 Contaminant Transport and Transformation
   3.2 Identification of Principal Pathways of Exposure
   3.3 Estimates of Environmental Concentrations

4. Exposed Populations Analysis

   4.1 Exposed population identification
      - Individual exposure points
   4.2 Exposed population enumeration
      - Individual exposure points
   4.3 Exposed population characterization
      - General population
      - Sensitive subpopulations

5. Exposure Calculation and Integration

   5.1 Development of medium-specific exposure estimates for each hazardous substance and for each exposed population segment
   5.2 Exposure Integration

6. Uncertainty in the Assessment

7. References

8. Appendices

   A. Completed data management forms

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 [illegible]

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 (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.				

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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.					
6.					

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
7.				
8.				
9.				
10.				

Form #5: Short-term Exposure Calculation

Site Name: _____
Date: _____
Analyst: _____

1 Chemical	2 Exposure Mechanism	3 Short-term Exposure per Event (units)	4 Events per Time Period	5 Body Mass (kg)	6 Time Period (days)	7 Short-term Daily Exposure (mg/kg/day) [3x4÷5x6]	8 Exposed Population Segment (number of persons)
1.							
2.							
3.							
4.							
5.							

Form #5: Short-term Exposure Calculation (continued)

Site Name: _____
Date: _____
Analyst: _____

1 Chemical	2 Exposure Mechanism	3 Short-term Exposure per Event (units)	4 Events per Time Period	5 Body Mass (kg)	6 Time Period (days)	7 Short-term Daily Exposure (mg/kg/day) [3x4÷5x6]	8 Exposed Population Segment (number of persons)
6.							
7.							
8.							
9.							
10.							

Form #6: Long-term Exposure Calculation

Site Name: _____
Date: _____
Analyst: _____

1 Chemical	2 Exposure Mechanism	3 Long-term Exposure per Event (units)	4 Events per Time Period	5 Body Mass (kg)	6 Time Period (2.56×10^4 days)	7 Long-term Daily Exposure (mg/kg/day) [3x4÷5x6]	8 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) [3x4÷5x6]	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. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	6. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	7. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____

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Region V, Library
230 South Dearborn Street
Chicago, Illinois 60604

Form #7: E[illegible]ure Integration (continued)

Site Name: _____
Date: _____
Analyst: _____

Population Segment	Chemical	Exposure Mechanism	Exposure Short-term	Exposure Long-term	Number exposed
	8. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	9. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
	10. _____	_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____
		_____	_____	_____	_____