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Office of Solid Waste and
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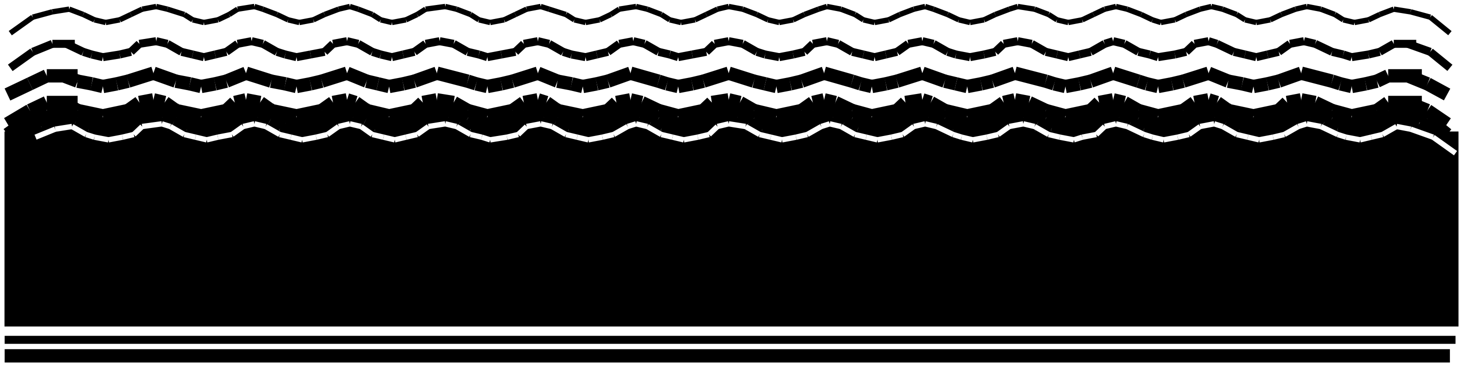
Superfund

Soil Screening Guidance: Technical Background Document

Second Edition



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DISCLAIMER

Notice: The Soil Screening Guidance is based on policies set out in the Preamble to the Final Rule of the National Oil and Hazardous Substances Pollution Contingency Plan (NCP), which was published on March 8, 1990 (55 *Federal Register* 8666).

This guidance document sets forth recommended approaches based on EPA's best thinking to date with respect to soil screening. Alternative approaches for screening may be found to be more appropriate at specific sites (e.g., where site circumstances do not match the underlying assumptions, conditions, and models of the guidance). The decision whether to use an alternative approach and a description of any such approach should be placed in the Administrative Record for the site.

The policies set out in both the Soil Screening Guidance: User's Guide and the supporting Soil Screening Guidance: Technical Background Document are intended solely as guidance to the U.S. Environmental Protection Agency (EPA) personnel; they are not final EPA actions and do not constitute rulemaking. These policies are not intended, nor can they be relied upon, to create any rights enforceable by any party in litigation with the United States government. EPA officials may decide to follow the guidance provided in this document, or to act at variance with the guidance, based on an analysis of specific site circumstances. EPA also reserves the right to change the guidance at any time without public notice.

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PREFACE

This document provides the technical background for the development of methodologies described in the *Soil Screening Guidance: User's Guide* (EPA/540/R-96/018), along with additional information useful for soil screening. Together, these documents define the framework and methodology for developing Soil Screening Levels (SSLs) for chemicals commonly found at Superfund sites. This document is an updated version of the background document developed in support of the December 30, 1994, draft Soil Screening Guidance. The methodologies described in this document and the guidance have been revised in response to public comment and extensive peer review. The revisions, along with other technical analyses conducted to address the comments, are described herein.

This background document is presented in five parts. Part 1 describes the soil screening process and its application and implementation at Superfund sites. Part 2 describes the methodology used to develop SSLs, including the assumptions and theories used. Part 3 provides information on more detailed models that may be used to develop site-specific SSLs. Part 4 addresses sampling schemes for measuring soil contaminant levels during the soil screening process. Part 5 provides technical background on the determination of chemical-specific properties for calculating SSLs.

ACKNOWLEDGMENTS

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Part 1: INTRODUCTION

This document provides the technical background for the Soil Screening Guidance. The Soil Screening Guidance is a tool that the U.S. Environmental Protection Agency (EPA) developed to help standardize and accelerate the evaluation and cleanup of contaminated soils at sites on the National Priorities List (NPL) with anticipated future residential land use scenarios.[1] This guidance provides a methodology for environmental science/engineering professionals to calculate risk-based, site-specific, soil screening levels (SSLs), for contaminants in soil that may be used to identify areas needing further investigation at NPL sites.

SSLs are not national cleanup standards. SSLs alone do not trigger the need for response actions or define "unacceptable" levels of contaminants in soil. "Screening," for the purposes of this guidance, refers to the process of identifying and defining areas, contaminants, and conditions at a particular site that do not require further Federal attention. Generally, at sites where contaminant concentrations fall below SSLs, no further action or study is warranted under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA). (Some States have developed screening numbers or methodologies that may be more stringent than SSLs; therefore further study may be warranted under State programs.) Where contaminant concentrations equal or exceed the SSLs, further study or investigation, but not necessarily cleanup, is warranted.

The Soil Screening Guidance provides a framework for screening contaminated soils that encompasses both simple and more detailed approaches for calculating site-specific SSLs, and generic SSLs for use where site-specific data are limited. The *Soil Screening Guidance: User's Guide* (U.S. EPA, 1996) focuses on the application of the simple site-specific approach by providing a step-by-step methodology to calculate site-specific SSLs and plan the sampling necessary to apply them. This Technical Background Document describes the development and technical basis of the methodology presented in the User’s Guide. It includes detailed modeling approaches for developing screening levels that can take into account more complex site conditions than the simple site-specific methodology emphasized in the User's Guide. It also provides generic SSLs for the most common contaminants found at NPL sites.

1.1 Background

The Soil Screening Guidance is the result of technical analyses and coordination with numerous stakeholders. The effort began in 1991 when the EPA Administrator charged the Office of Solid Waste and Emergency Response (OSWER) with conducting a 30-day study to outline options for accelerating the rate of cleanups at NPL sites. One of the specific proposals of the study was for OSWER to "examine the means to develop standards or guidelines for contaminated soils." Over the past 4 years, several drafts of the guidance and the accompanying technical background document have had widespread reviews both within and outside EPA. In the Spring of 1995, final drafts were released for public comment and external scientific peer review. Many reviewers' comments contributed significantly to the development of this flexible tool that uses site-specific data in a methodology that can be applied consistently across the nation.

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[1] Note that the Superfund program defines “soil” as having a particle size under 2 millimeters, while the RCRA program allows for particles under 9 millimeters in size.

1.2 Purpose of SSLs

In identifying and managing risks at sites, EPA considers a spectrum of contaminant concentrations. The level of concern associated with those concentrations depends on the likelihood of exposure to soil contamination at levels of potential concern to human health or to ecological receptors. Figure 1 illustrates the spectrum of soil contamination encountered at Superfund sites and the conceptual range of risk management. At one end are levels of contamination that clearly warrant a response action; at the other end are levels that are below regulatory concern. Appropriate cleanup goals for a particular site may fall anywhere within this range depending on site-specific conditions. Screening levels identify the lower bound of the spectrum -- levels below which there is no concern under CERCLA, provided conditions associated with the SSLs are met.

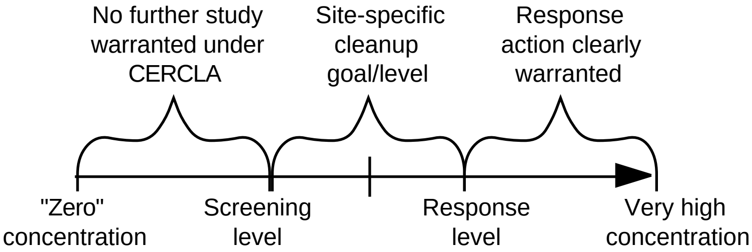


Figure 1. Conceptual Risk Management Spectrum for Contaminated Soil

Although the application of SSLs during site investigations is not mandatory at sites being addressed by CERCLA or RCRA, EPA recommends the use of SSLs as a tool to facilitate prompt identification of contaminants and exposure areas of concern. EPA developed the Soil Screening Guidance to be consistent with and to enhance the current Superfund investigation process and anticipates its primary use during the early stages of a remedial investigation (RI) at NPL sites. It does not replace the Remedial Investigation/Feasibility Study (RI/FS) or risk assessment, but use of screening levels can focus the RI and risk assessment on aspects of the site that are more likely to be a concern under CERCLA. By screening out areas of sites, potential chemicals of concern, or exposure pathways from further investigation, site managers and technical experts can limit the scope of the remedial investigation or risk assessment. SSLs can save resources by helping to determine which areas do not require additional Federal attention early in the process. Furthermore, data gathered during the soil screening process can be used in later Superfund phases, such as the baseline risk assessment, feasibility study, treatability study, and remedial design. This guidance may also be appropriate for use by the removal program when demarcation of soils above residential risk-based numbers coincides with the purpose and scope of the removal action. EPA created the Soil Screening Guidance to be consistent with and to enhance current Superfund processes.

The process presented in this guidance to develop and apply simple, site-specific soil screening levels is likely to be most useful where it is difficult to determine whether areas of soil are contaminated to an extent that warrants further investigation or response (e.g., whether areas of soil at an NPL site require further investigation under CERCLA through an RI/FS). The screening levels have been developed assuming future residential land use assumptions and related exposure scenarios. Although some of the models and methods presented in this guidance could be modified to address exposures under other land uses, EPA has not yet standardized assumptions for those other uses. Using this guidance for sites where residential land use assumptions do not apply could result in overly conservative screening levels. However, EPA recognizes that some parties responsible for sites with non-residential land use might still benefit from using SSLs as a tool to conduct conservative initial screening.

EPA created the *Soil Screening Guidance: User's Guide* (U.S. EPA, 1996) to be easy to use: it provides a simple step-by-step methodology for calculating SSLs that are specific to the user's site. Applying site-specific screening levels involves developing a conceptual site model (CSM), collecting a few easily obtained site-specific soil parameters (such as the dry bulk density and percent soil moisture), and sampling soil to measure contaminant levels in surface and subsurface soils. Often, much of the information needed to develop the CSM can be derived from previous site investigations (e.g., the preliminary assessment/site inspection [PA/SI]) and, if properly planned, SSL sampling can be accomplished in one mobilization.

SSLs can be used as Preliminary Remediation Goals (PRGs) provided appropriate conditions are met (i.e., conditions found at a specific site are similar to conditions assumed in developing the SSLs). The concept of calculating risk-based soil levels for use as PRGs (or "draft" cleanup levels) was introduced in the *Risk Assessment Guidance for Superfund* (RAGS)*, Volume I, Human Health Evaluation Manual* (HHEM)*, Part B* (U.S. EPA, 1991b). PRGs are risk-based values that provide a reference point for establishing site-specific cleanup levels. The models, equations, and assumptions presented in the Soil Screening Guidance and described herein to address inhalation exposures supersede those described in RAGS HHEM, Part B, for residential soils. **In addition, this guidance presents methodologies to address the leaching of contaminants through soil to an underlying potable aquifer. This pathway should be addressed in the development of PRGs.**

EPA emphasizes that SSLs are **not** cleanup standards. SSLs should not be used as site-specific cleanup levels unless a site-specific nine-criteria evaluation using SSLs as PRGs for soils indicates that a selected remedy achieving the SSLs is protective, compliant with applicable or relevant and appropriate requirements (ARARs), and appropriately balances the other criteria, including cost. PRGs may then be converted into final cleanup levels based on the nine-criteria analysis described in the National Contingency Plan (NCP; Section 300.430 (3)(2)(A)). The directive entitled *Role of the Baseline Risk Assessment in Superfund Remedy Selection Decisions* (U.S. EPA, 1991c) discusses the modification of PRGs to generate cleanup levels.

The generic SSLs provided in Appendix A are calculated from the same equations used in the simple site-specific methodology, but are based on a number of default assumptions chosen to be protective of human health for most site conditions. Generic SSLs can be used in place of site-specific screening levels; however, they are expected to be generally more conservative than site-specific levels. The site manager should weigh the cost of collecting the data necessary to develop site-specific SSLs with the potential for deriving a higher SSL that provides an appropriate level of protection.

1.3 Scope of Soil Screening Guidance

The Soil Screening Guidance incorporates readily obtainable site data into simple, standardized equations to derive site-specific screening levels for selected contaminants and exposure pathways. Key attributes of the Soil Screening Guidance are given in Highlight 1.

Highlight 1: Key Attributes of the Soil Screening Guidance

- Standardized equations are presented to address human exposure pathways in a residential setting consistent with Superfund's concept of "Reasonable Maximum Exposure" (RME).
- Source size (area and depth) can be considered on a site-specific basis using mass-limit models.
- Parameters are identified for which site-specific information is needed to develop site-specific SSLs.
- Default values are provided to calculate generic SSLs where site-specific information is not available.
- SSLs are generally based on a 10^{-6} risk for carcinogens, or a hazard quotient of 1 for noncarcinogens; SSLs for migration to ground water are based on (in order of preference): nonzero maximum contaminant level goals (MCLGs), maximum contaminant levels (MCLs), or the aforementioned risk-based targets.

1.3.1 Exposure Pathways. In a residential setting, potential pathways of exposure to contaminants in soil are as follows (see Figure 2):

- Direct ingestion
- Inhalation of volatiles and fugitive dusts
- Ingestion of contaminated ground water caused by migration of chemicals through soil to an underlying potable aquifer
- Dermal absorption
- Ingestion of homegrown produce that has been contaminated via plant uptake
- Migration of volatiles into basements

The Soil Screening Guidance addresses each of these pathways to the greatest extent practical. The first three pathways -- direct ingestion, inhalation of volatiles and fugitive dusts, and ingestion of potable ground water, are the most common routes of human exposure to contaminants in the residential setting. These pathways have generally accepted methods, models, and assumptions that lend themselves to a standardized approach. The additional pathways of exposure to soil contaminants, dermal absorption, plant uptake, and migration of volatiles into basements, may also contribute to the risk to human health from exposure to specific contaminants in a residential setting. This guidance addresses these pathways to a limited extent based on available empirical data (see Part 2 for further discussion).

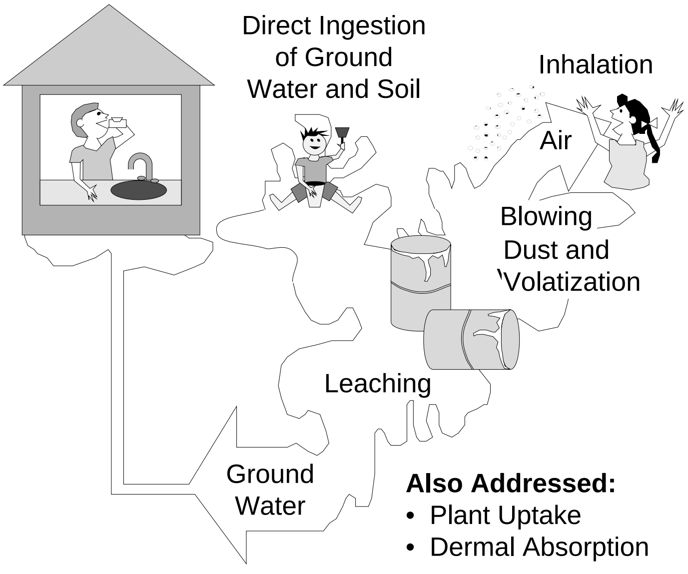


Figure 2. Exposure Pathways Addressed by SSLs.

The Soil Screening Guidance addresses the human exposure pathways listed previously and will be appropriate for most residential settings. The presence of additional pathways or unusual site conditions does not preclude the use of SSLs in areas of the site that are currently residential or likely to be residential in the future. However, the risks associated with these additional pathways or conditions (e.g., fish consumption, raising of livestock, heavy truck traffic on unpaved roads) should be considered in the remedial investigation/feasibility study (RI/FS) to determine whether SSLs are adequately protective.

An ecological assessment should also be performed as part of the RI/FS to evaluate potential risks to ecological receptors.

The Soil Screening Guidance should not be used for areas with radioactive contaminants.

1.3.2 Exposure Assumptions. SSLs are risk-based concentrations derived from equations combining exposure assumptions with EPA toxicity data. The models and assumptions used to calculate SSLs were developed to be consistent with Superfund's concept of "reasonable maximum exposure" (RME) in the residential setting. The Superfund program's method to estimate the RME for chronic exposures on a site-specific basis is to combine an average exposure point concentration with reasonably conservative values for intake and duration in the exposure calculations (U.S. EPA, 1989b; U.S. EPA, 1991a). The default intake and duration assumptions presented in U.S. EPA (1991a) were chosen to represent individuals living in a small town or other nontransient community. (Exposure to members of a more transient community is assumed to be shorter and thus associated with lower risk.) Exposure point concentrations are either measured at the site (e.g., ground water concentrations at a receptor well) or estimated using exposure models with site-specific model inputs. An average concentration term is used in most assessments where the focus is on estimating long-term, chronic exposures. Where the potential for acute toxicity is of concern, exposure estimates based on maximum concentrations may be more appropriate.

The resulting site-specific estimate of RME is then compared with a chemical-specific toxicity criterion such as a reference dose (RfD) or a reference concentration (RfC). EPA recommends using criteria from the Integrated Risk Information System (IRIS) (U.S. EPA, 1995b) and Health Effects Assessment Summary Tables (HEAST) (U.S. EPA, 1995d), although values from other sources may be used in appropriate cases.

SSLs are concentrations of contaminants in soil that are designed to be protective of exposures in a residential setting. A site-specific risk assessment is an evaluation of the risk posed by exposure to site contaminants in various media. To calculate SSLs, the exposure equations and pathway models are run in reverse to backcalculate an “acceptable level” of a contaminant in soil corresponding to a specific level of risk.

1.3.3 Risk Level. For the ingestion, dermal, and inhalation pathways, toxicity criteria are used to define an acceptable level of contamination in soil, based on a one-in-a-million (10^{-6}) individual excess cancer risk for carcinogens and a hazard quotient (HQ) of 1 for non-carcinogens. SSLs are backcalculated for migration to ground water pathways using ground water concentration limits [nonzero maximum contaminant level goals (MCLGs), maximum contaminant levels (MCLs), or health-based limits (HBLs) (10^{-6} cancer risk or a HQ of 1) where MCLs are not available].

The potential for additive effects has not been "built in" to the SSLs through apportionment. For carcinogens, EPA believes that setting a 10^{-6} risk level for individual chemicals and pathways will generally lead to cumulative risks within the risk range (10^{-4} to 10^{-6}) for the combinations of chemicals typically found at Superfund sites. For noncarcinogens, additive risks should be considered only for those chemicals with the same toxic endpoint or mechanism of action (see Section 2.1).

1.3.4 SSL Model Assumptions. The models used to calculate inhalation and migration to ground water SSLs were designed for use at an early stage of site investigation when site information may be limited. Because of this constraint, they incorporate a number of simplifying assumptions.

The models assume that the source is infinite. Although the assumption is highly conservative, a finite source model cannot be applied unless there are accurate data regarding source size and volume. EPA believes it to be unlikely that such data will be available from the limited subsurface sampling that is done to apply SSLs. However, EPA also recognizes that infinite source models can violate mass balance (i.e., can release more contaminants than are present) for certain contaminants and site conditions (e.g., small sources). To address this problem, this guidance includes simple models that provide a mass-based limit for the inhalation and migration to ground water SSLs (see Section 2.6). **A site-specific estimate of source depth and area are required to calculate SSLs using these models**.

The infinite source assumption leads to several other simplifying assumptions. Fractionation of contaminant mass between the inhalation and migration to ground water pathways cannot be addressed with infinite source models. For the migration to ground water pathway, an infinite source overrides adsorption in the unsaturated zone or in the aquifer. The models also assume that contamination is evenly distributed throughout the source (i.e., homogeneous) and that no biological or chemical degradation occurs in the soil or in the aquifer. Again, models capable of addressing heterogeneities or degradation processes require collection of site-specific data that is well beyond the scope of the Soil Screening Guidance.

Although the Soil Screening Guidance encourages the use of site-specific data to calculate SSLs, conservative default parameters are provided for use where site-specific data are not available. These defaults are described in Part 2 of this document. Appendix A provides an example set of "generic" SSLs for 110 chemicals that are calculated using these defaults. Because they are designed to be protective of most site conditions across the nation, they are conservative.

A default 0.5 acre source area is used to calculate the generic SSLs. A 30 acre source size was used in the December 1994 guidance. EPA received an overwhelming number of comments that suggest that most contaminated soil sources addressed under the Superfund program are 0.5 acres or smaller. Because of the infinite source assumption, generic SSLs based on a 0.5 acre source size can be protective of larger sources as well (see Appendix A). However, this hypothesis should be examined on a case-by-case basis before applying the generic SSLs to sources larger than 0.5 acre.

1.4 Organization of the Document

Part 2 of this document describes the development of the simple equations used to calculate SSLs. It describes and supports the assumptions behind these equations and presents the results of analyses conducted to develop the SSL methodology. Some of the more sensitive parameters are identified for which site-specific data are likely to have a significant impact. Default values are provided along with their sources and limitations.

Part 3 presents information on other, more complex models that can be used to calculate inhalation and migration to ground water SSLs when more extensive site data are available or can be obtained.

Some of these models can consider a finite source and fractionation between exposure pathways. They also can model more complex site conditions than the simple SSL equations, including conditions that can lead to higher, yet still protective, SSLs (e.g., thick unsaturated zones, biological and chemical degradation, layered soils).

Part 4 provides the technical background for the development of the soil sampling design methodology for SSL application. It addresses methods for surface soil, including a test based on a maximum soil composite sample and the Chen method, which allows decision errors to be controlled. Part 4 also provides simulation results that measure the performance of these methods and sample size tables for different contaminant distributions and compositing schemes. Step-by-step guidance is provided for developing sample designs using each statistical procedure.

Part 5 describes the selection and development of the chemical properties used to calculate SSLs.

Part 2: DEVELOPMENT OF PATHWAY-SPECIFIC SOIL SCREENING LEVELS

This part of the Technical Background Document describes the methods used to calculate SSLs for residential exposure pathways, along with their technical basis and limitations associated with their use. Simple, standardized equations have been developed for three common exposure pathways at Superfund sites:

- Ingestion of soil (Section 2.2)
- Inhalation of volatiles and fugitive dust (Section 2.4)
- Ingestion of contaminated ground water caused by migration of contaminants through soil to an underlying potable aquifer (Section 2.5).

The equations were developed under the following constraints:

- They should be consistent with current Superfund risk assessment methodologies and guidance.
- To be appropriate for early-stage application, they should be simple and easy to apply.
- They should allow the use of site-specific data where they are readily available or can be easily obtained.
- The process of developing and applying SSLs should generate information that can be used and built upon as a site evaluation progresses.

The equations for the inhalation and migration to ground water pathways include easily obtained site-specific input parameters. Conservative default values have been developed for use where site-specific data are not available. Generic SSLs, calculated for 110 chemicals using these default values, are presented in Appendix A. The generic SSLs are conservative, since the default values are designed to be protective at most sites across the country.

The inhalation and migration to ground water pathway equations assume an infinite source. As pointed out by several commenters to the December 1994 draft Soil Screening Guidance (U.S. EPA, 1994h), SSLs developed using these models may violate mass-balance for certain contaminants and site conditions (e.g., small sources). To address this concern, EPA has incorporated simple mass-limit models for these pathways assuming that the entire volume of contamination either volatilizes or leaches over the duration of exposure and that the level of contaminant at the receptor does not exceed the health-based limit (Section 2.6). **Because they require a site-specific estimate of source depth, these models cannot be used to calculate generic SSLs.**

Dermal adsorption, consumption of garden vegetables grown in contaminated soil, and migration of volatiles into basements also may contribute significantly to the risk to human health from exposure to soil contaminants in a residential setting. These pathways have been incorporated into the Soil Screening Guidance to the greatest extent practical.

Although methods for quantifying dermal exposures are available, their use for calculating SSLs is limited by the amount of data available on dermal absorption of specific chemicals (Section 2.3). Screening equations have been developed to estimate human exposure from the uptake of soil contaminants by garden plants (Section 2.7). As with dermal absorption, the number of chemicals for which adequate empirical data on plant uptake are limited. An approach to address migration of volatiles into basements is presented in Section 2.8, and limitations of the approach are discussed.

Section 2.1 describes the human health basis of the Soil Screening Guidance and provides the human toxicity and health benchmarks necessary to calculate SSLs. The selection and development of the chemical properties required to calculate SSLs are described in Part 5 of this document.

2.1 Human Health Basis

Table 1 lists the regulatory and human health benchmarks necessary to calculate SSLs for 110 chemicals including:

- Ingestion SSLs: oral cancer slope factors (SF_o) and noncancer reference doses (RfDs)
- Inhalation SSLs: inhalation unit risk factors (URFs) and reference concentrations (RfCs)
- Migration to ground water SSLs: drinking water standards (MCLGs and MCLs) and drinking water health-based levels (HBLs).

The human health benchmarks in Table 1 were obtained from IRIS (U.S. EPA, 1995b) or HEAST (U.S. EPA, 1995d) unless otherwise indicated. MCLGs and MCLs were obtained from U.S. EPA (1995a). Each of these references is updated regularly. **Prior to calculating SSLs, the values in Table 1 should be checked against the most recent version of these sources to ensure that they are up-to-date.**

2.1.1 Additive Risk. For soil ingestion and inhalation of volatiles and fugitive dusts, SSLs correspond to a 10^{-6} risk level for carcinogens and a hazard quotient of 1 for noncarcinogens. For carcinogens, EPA believes that setting a 10^{-6} risk level for individual chemicals and pathways generally will lead to cumulative risks within the 10^{-4} to 10^{-6} range for the combinations of chemicals typically found at Superfund sites.

Whereas the carcinogenic risks of multiple chemicals are simply added together, the issue of additive risk is much more complex for noncarcinogens because of the theory that a threshold exists for noncancer effects. This threshold level, below which adverse effects are not expected to occur, is the basis for EPA's RfD and RfC. Since adverse effects are not expected to occur at the RfD or RfC and the SSLs were derived by setting the potential exposure dose equal to the RfD or RfC (i.e., an HQ equal to 1), it is difficult to address the risk of exposure to multiple chemicals at levels where the individual chemicals alone would not be expected to cause any harmful effect. However, problems may arise when multiple chemicals produce related toxic effects.

EPA believes, and the Science Advisory Board (SAB) agrees (U.S. EPA, 1993e), that HQs should be added only for those chemicals with the same toxic endpoint and/or mechanism of action.

Table 1. Regulatory and Human Health Benchmarks Used for SSL Development

		Maximum Contaminant Level Goal (mg/L)		Maximum Contaminant Level (mg/L)		Water Health Based Limits (mg/L)		Cancer Slope Factor $(mg/kg\text{-}d)^{-1}$			Unit Risk Factor $(\mu g/m^3)^{-1}$			Reference Dose (mg/kg-d)		Reference Concentration (mg/m^3)	
CAS Number	**Chemical Name**	**MCLG (PMCLG)**	**Ref.** [a]	**MCL (PMCL)**	**Ref.** [a]	**HBL** [b]	**Basis**	**Carc. Class** [c]	SF_o	**Ref.** [a]	**Carc. Class** [c]	**URF**	**Ref.** [a]	**RfD**	**Ref.** [a]	**RfC**	**Ref.** [a]
83-32-9	Acenaphthene					2E+00	RfD							6.0E-02	1		
67-64-1	Acetone (2-Propanone)					4E+00	RfD	D			D			1.0E-01	1		
309-00-2	Aldrin					5E-06	SF_o	B2	1.7E+01	1	B2	4.9E-03	1	3.0E-05	1		
120-12-7	Anthracene					1E+01	RfD	D			D			3.0E-01	1		
7440-36-0	Antimony	6.0E-03	3	6.0E-03	3									4.0E-04	1		
7440-38-2	Arsenic			5.0E-02	3			A	1.5E+00	1	A	4.3E-03	1	3.0E-04	1		
7440-39-3	Barium	2.0E+00	3	2.0E+00	3									7.0E-02	1	5.0E-04	2
56-55-3	Benz(*a*)anthracene					1E-04	SF_o	B2	7.3E-01	4	B2						
71-43-2	Benzene			5.0E-03	3			A	2.9E-02	1	A	8.3E-06	1				
205-99-2	Benzo(*b*)fluoranthene					1E-04	SF_o	B2	7.3E-01	4	B2						
207-08-9	Benzo(*k*)fluoranthene					1E-03	SF_o	B2	7.3E-02	4	B2						
65-85-0	Benzoic acid					1E+02	RfD							4.0E+00	1		
50-32-8	Benzo(*a*)pyrene			2.0E-04	3			B2	7.3E+00	1	B2						
7440-41-7	Beryllium	4.0E-03	3	4.0E-03	3			B2	4.3E+00	1	B2	2.4E-03	1	5.0E-03	1		
111-44-4	Bis(2-chloroethyl)ether					8E-05	SF_o	B2	1.1E+00	1	B2	3.3E-04	1				
117-81-7	Bis(2-ethylhexyl)phthalate			6.0E-03	3			B2	1.4E-02	1	B2			2.0E-02	1		
75-27-4	Bromodichloromethane			1.0E-01 *	3			B2	6.2E-02	1	B2			2.0E-02	1		
75-25-2	Bromoform (tribromomethane)			1.0E-01 *	3			B2	7.9E-03	1	B2	1.1E-06	1	2.0E-02	1		
71-36-3	Butanol					4E+00	RfD	D			D			1.0E-01	1		
85-68-7	Butyl benzyl phthalate					7E+00	RfD	C			C			2.0E-01	1		
7440-43-9	Cadmium	5.0E-03	3	5.0E-03	3						B1	1.8E-03	1	1.0E-03**	1		
86-74-8	Carbazole					4E-03	SF_o	B2	2.0E-02	2							
75-15-0	Carbon disulfide					4E+00	RfD							1.0E-01	1	7.0E-01	1
56-23-5	Carbon tetrachloride			5.0E-03	3			B2	1.3E-01	1	B2	1.5E-05	1	7.0E-04	1		
57-74-9	Chlordane			2.0E-03	3			B2	1.3E+00	1	B2	3.7E-04	1	6.0E-05	1		
106-47-8	*p* -Chloroaniline					1E-01	RfD							4.0E-03	1		
108-90-7	Chlorobenzene	1.0E-01	3	1.0E-01	3			D			D			2.0E-02	1	2.0E-02	2
124-48-1	Chlorodibromomethane	6.0E-02	3	1.0E-01 *	3			C	8.4E-02	1	C			2.0E-02	1		
67-66-3	Chloroform			1.0E-01 *	3			B2	6.1E-03	1	B2	2.3E-05	1	1.0E-02	1		
95-57-8	2-Chlorophenol					2E-01	RfD							5.0E-03	1		

* Proposed MCL = 0.08 mg/L, *Drinking Water Regulations and Health Advisories* , U.S. EPA (1995).

** Cadmium RfD is based on dietary exposure.

Table 1 (continued)

		Maximum Contaminant Level Goal (mg/L)		Maximum Contaminant Level (mg/L)		Water Health Based Limits (mg/L)		Cancer Slope Factor $(mg/kg\text{-}d)^{-1}$			Unit Risk Factor $(\mu g/m^3)^{-1}$			Reference Dose (mg/kg-d)		Reference Concentration (mg/m^3)	
CAS Number	Chemical Name	MCLG (PMCLG)	Ref. ^{a}	MCL (PMCL)	Ref. ^{a}	HBL ^{b}	Basis	Carc. Class ^{c}	SF_o	Ref. ^{a}	Carc. Class ^{c}	URF	Ref. ^{a}	RfD	Ref. ^{a}	RfC	Ref. ^{a}
7440-47-3	Chromium	1.0E-01	3	1.0E-01	3			A			A	1.2E-02	1	5.0E-03	1		
16065-83-1	Chromium (III)					4E+01	RfD							1.0E+00	1		
18540-29-9	Chromium (VI)			1.0E-01	3 *			A			A	1.2E-02	1	5.0E-03	1		
218-01-9	Chrysene					1E-02	SF_o	B2	7.3E-03	4							
57-12-5	Cyanide (amenable)	(2.0E-01)	3	(2.0E-01)	3			D			D			2.0E-02	1		
72-54-8	DDD					4E-04	SF_o	B2	2.4E-01	1	B2						
72-55-9	DDE					3E-04	SF_o	B2	3.4E-01	1	B2						
50-29-3	DDT					3E-04	SF_o	B2	3.4E-01	1	B2	9.7E-05	1	5.0E-04	1		
53-70-3	Dibenz(*a,h*)anthracene					1E-05	SF_o	B2	7.3E+00	4	B2						
84-74-2	Di-*n* -butyl phthalate					4E+00	RfD	D			D			1.0E-01	1		
95-50-1	1,2-Dichlorobenzene	6.0E-01	3	6.0E-01	3			D			D			9.0E-02	1	2.0E-01	2
106-46-7	1,4-Dichlorobenzene	7.5E-02	3	7.5E-02	3			B2	2.4E-02	2	B2					8.0E-01	1
91-94-1	3,3-Dichlorobenzidine					2E-04	SF_o	B2	4.5E-01	1	B2						
75-34-3	1,1-Dichloroethane					4E+00	RfD	C			C			1.0E-01	7	5.0E-01	2
107-06-2	1,2-Dichloroethane			5.0E-03	3			B2	9.1E-02	1	B2	2.6E-05	1				
75-35-4	1,1-Dichloroethylene	7.0E-03	3	7.0E-03	3			C	6.0E-01	1	C	5.0E-05	1	9.0E-03	1		
156-59-2	*cis* -1,2-Dichloroethylene	7.0E-02	3	7.0E-02	3			D			D			1.0E-02	2		
156-60-5	*trans* -1,2-Dichloroethylene	1.0E-01	3	1.0E-01	3									2.0E-02	1		
120-83-2	2,4-Dichlorophenol					1E-01	RfD							3.0E-03	1		
78-87-5	1,2-Dichloropropane			5.0E-03	3			B2	6.8E-02	2	B2					4.0E-03	1
542-75-6	1,3-Dichloropropene					5E-04	SF_o	B2	1.8E-01	2	B2	3.7E-05	2	3.0E-04	1	2.0E-02	1
60-57-1	Dieldrin					5E-06	SF_o	B2	1.6E+01	1	B2	4.6E-03	1	5.0E-05	1		
84-66-2	Diethylphthalate					3E+01	RfD	D			D			8.0E-01	1		
105-67-9	2,4-Dimethylphenol					7E-01	RfD							2.0E-02	1		
51-28-5	2,4-Dinitrophenol					4E-02	RfD							2.0E-03	1		
121-14-2	2,4-Dinitrotoluene**					1E-04	SF_o	B2	6.8E-01	1				2.0E-03	1		
606-20-2	2,6-Dinitrotoluene**					1E-04	SF_o	B2	6.8E-01	1				1.0E-03	2		
117-84-0	Di-*n* -octyl phthalate					7E-01	RfD							2.0E-02	2		
115-29-7	Endosulfan					2E-01	RfD							6.0E-03	2		
72-20-8	Endrin	2.0E-03	3	2.0E-03	3			D			D			3.0E-04	1		

* MCL for total chromium is based on Cr (VI) toxicity.

** Cancer Slope Factor is for 2,4-, 2,6-Dinitrotoluene mixture.

Table 1 (continued)

		Maximum Contaminant Level Goal (mg/L)		Maximum Contaminant Level (mg/L)		Water Health Based Limits (mg/L)		Cancer Slope Factor (mg/kg-d)$^{-1}$			Unit Risk Factor (µg/m^3)$^{-1}$			Reference Dose (mg/kg-d)		Reference Concentration (mg/m^3)	
CAS Number	**Chemical Name**	**MCLG (PMCLG)**	**Ref. [a]**	**MCL (PMCL)**	**Ref. [a]**	**HBL [b]**	**Basis**	**Carc. Class [c]**	**SF_o**	**Ref. [a]**	**Carc. Class [c]**	**URF**	**Ref. [a]**	**RfD**	**Ref. [a]**	**RfC**	**Ref. [a]**
100-41-4	Ethylbenzene	7.0E-01	3	7.0E-01	3			D			D			1.0E-01	1	1.0E+00	1
206-44-0	Fluoranthene					1E+00	RfD	D			D			4.0E-02	1		
86-73-7	Fluorene					1E+00	RfD	D						4.0E-02	1		
76-44-8	Heptachlor			4.0E-04	3			B2	4.5E+00	1	B2	1.3E-03	1	5.0E-04	1		
1024-57-3	Heptachlor epoxide			2.0E-04	3			B2	9.1E+00	1	B2	2.6E-03	1	1.3E-05	1		
118-74-1	Hexachlorobenzene			1.0E-03	3			B2	1.6E+00	1	B2	4.6E-04	1	8.0E-04	1		
87-68-3	Hexachloro-1,3-butadiene	1.0E-03	3			1E-03	SF_o	C	7.8E-02	1	C	2.2E-05	1	2.0E-04	2		
319-84-6	α-HCH (α-BHC)					1E-05	SF_o	B2	6.3E+00	1	B2	1.8E-03	1				
319-85-7	β-HCH (β-BHC)					5E-05	SF_o	C	1.8E+00	1	C	5.3E-04	1				
58-89-9	γ-HCH (Lindane)	2.0E-04	3	2.0E-04	3			B2	1.3E+00	2	C			3.0E-04	1		
77-47-4	Hexachlorocyclopentadiene	5.0E-02	3	5.0E-02	3			D			D			7.0E-03	1	7.0E-05	2
67-72-1	Hexachloroethane					6E-03	SF_o	C	1.4E-02	1	C	4.0E-06	1	1.0E-03	1		
193-39-5	Indeno(1,2,3-*cd*)pyrene					1E-04	SF_o	B2	7.3E-01	4	B2						
78-59-1	Isophorone					9E-02	SF_o	C	9.5E-04	1	C			2.0E-01	1		
7439-97-6	Mercury	2.0E-03	3	2.0E-03	3			D			D			3.0E-04	2	3.0E-04	2
72-43-5	Methoxychlor	4.0E-02	3	4.0E-02	3			D			D			5.0E-03	1		
74-83-9	Methyl bromide					5E-02	RfD	D			D			1.4E-03	1	5.0E-03	1
75-09-2	Methylene chloride			5.0E-03	3			B2	7.5E-03	1	B2	4.7E-07	1	6.0E-02	1	3.0E+00	2
95-48-7	2-Methylphenol (*o* -cresol)					2E+00	RfD	C			C			5.0E-02	1		
91-20-3	Naphthalene					1E+00	RfD	D			D			4.0E-02	6		
7440-02-0	Nickel					1E-01	HA *	A			A	2.4E-04	1	2.0E-02	1		
98-95-3	Nitrobenzene					2E-02	RfD	D			D			5.0E-04	1	2.0E-03	2
86-30-6	*N* -Nitrosodiphenylamine					2E-02	SF_o	B2	4.9E-03	1	B2						
621-64-7	*N* -Nitrosodi-*n* -propylamine					1E-05	SF_o	B2	7.0E+00	1	B2						
87-86-5	Pentachlorophenol			1.0E-03	3			B2	1.2E-01	1	B2			3.0E-02	1		
108-95-2	Phenol					2E+01	RfD	D			D			6.0E-01	1		
129-00-0	Pyrene					1E+00	RfD	D			D			3.0E-02	1		
7782-49-2	Selenium	5.0E-02	3	5.0E-02	3			D			D			5.0E-03	1		
7440-22-4	Silver					2E-01	RfD	D			D			5.0E-03	1		
100-42-5	Styrene	1.0E-01	3	1.0E-01	3									2.0E-01	1	1.0E+00	1
79-34-5	1,1,2,2-Tetrachloroethane					4E-04	SF_o	C	2.0E-01	1	C	5.8E-05	1				

* Health advisory for nickel (MCL is currently remanded); EPA Office of Science and Technology, 7/10/95.

Table 1 (continued)

		Maximum Contaminant Level Goal (mg/L)		Maximum Contaminant Level (mg/L)		Water Health Based Limits (mg/L)		Cancer Slope Factor $(mg/kg\text{-}d)^{-1}$			Unit Risk Factor $(\mu g/m^3)^{-1}$			Reference Dose (mg/kg-d)		Reference Concentration (mg/m^3)	
CAS Number	Chemical Name	MCLG (PMCLG)	Ref. [a]	MCL (PMCL)	Ref. [a]	HBL [b]	Basis	Carc. Class [c]	SF_o	Ref. [a]	Carc. Class [c]	URF	Ref. [a]	RfD	Ref. [a]	RfC	Ref. [a]
127-18-4	Tetrachloroethylene			5.0E-03	3				5.2E-02	5		5.8E-07	5	1.0E-02	1		
7440-28-0	Thallium	5.0E-04	3	2.0E-03	3												
108-88-3	Toluene	1.0E+00	3	1.0E+00	3			D			D			2.0E-01	1	4.0E-01	1
8001-35-2	Toxaphene			3.0E-03	3			B2	1.1E+00	1	B2	3.2E-04	1				
120-82-1	1,2,4-Trichlorobenzene	7.0E-02	3	7.0E-02	3			D			D			1.0E-02	1	2.0E-01	2
71-55-6	1,1,1-Trichloroethane	2.0E-01	3	2.0E-01	3			D			D					1.0E+00	5
79-00-5	1,1,2-Trichloroethane	3.0E-03	3	5.0E-03	3			C	5.7E-02	1	C	1.6E-05	1	4.0E-03	1		
79-01-6	Trichloroethylene	zero	3	5.0E-03	3				1.1E-02	5		1.7E-06	5				
95-95-4	2,4,5-Trichlorophenol					4E+00	RfD							1.0E-01	1		
88-06-2	2,4,6-Trichlorophenol					8E-03	SF_o	B2	1.1E-02	1	B2	3.1E-06	1				
7440-62-2	Vanadium					3E-01	RfD							7.0E-03	2		
108-05-4	Vinyl acetate					4E+01	RfD							1.0E+00	1	2.0E-01	1
75-01-4	Vinyl chloride (chloroethene)			2.0E-03	3			A	1.9E+00	2	A	8.4E-05	2				
108-38-3	*m* -Xylene	1.0E+01	3 *	1.0E+01	3 *			D			D			2.0E+00	2		
95-47-6	*o* -Xylene	1.0E+01	3 *	1.0E+01	3 *			D			D			2.0E+00	2		
106-42-3	*p* -Xylene	1.0E+01	3 *	1.0E+01	3 *			D			D			2.0E+00	1 **		
7440-66-6	Zinc					1E+01	RfD	D			D			3.0E-01	1		

* MCL for total xylenes [1330-20-7] is 10 mg/L.

** RfD for total xylenes is 2 mg/kg-day.

[a] References:
1 = IRIS, U.S. EPA (1995b)
2 = HEAST, U.S. EPA (1995d)
3 = U.S. EPA (1995a)
4 = OHEA, U.S. EPA (1993c)
5 = Interim toxicity criteria provided by Superfund Health Risk Techincal Support Center, Environmental Criteria Assessment Office (ECAO), Cincinnati, OH (1994)
6 = ECAO, U.S. EPA (1994g)
7 = ECAO, U.S. EPA (1994f)

[b] Health Based Limits calculated for 30-year exposure duration, 10^{-6} risk or hazard quotient = 1.

[c] Categorization of overall weight of evidence for human carcinogenicity:

Group A:	human carcinogen
Group B:	probable human carcinogen
B1:	limited evidence from epidemiologic studies
B2:	"sufficient" evidence from animal studies and "inadequate" evidence or "no data" from epidemiologic studies
Group C:	possible human carcinogen
Group D:	not classifiable as to health carcinogenicity
Group E:	evidence of noncarcinogenicity for humans

Additivity of the SSLs for noncarcinogenic chemicals is further complicated by the fact that not all SSLs are based on toxicity. Some SSLs are determined instead by a "ceiling limit" concentration (C_{sat}) above which these chemicals may occur as nonaqueous phase liquids (NAPLs) in soil (see Section 2.4.4). Therefore, the potential for additive effects must be carefully evaluated at every site by considering the total Hazard Index (HI) for chemicals with RfDs or RfCs based on the same endpoint of toxicity (i.e., has the same critical effect as defined by the Reference Dose Methodology), excluding chemicals with SSLs based on C_{sat}. Table 2 lists several SSL chemicals with RfDs/RfCs, grouping those chemicals whose RfDs or RfCs are based on toxic effects in the same target organ or system. However, this list is limited, and a toxicologist should be consulted prior to addressing additive risks at a specific site.

2.1.2 Apportionment and Fractionation. EPA also has evaluated the SSLs for noncarcinogens in light of two related issues: apportionment and fractionation. **Apportionment** is typically used as the percentage of a regulatory health-based level that is allocated to the source/pathway being regulated (e.g., 20 percent of the RfD for the migration to ground water pathway). Apportioning risk assumes that the applied dose from the source, in this case contaminated soils, is only one portion of the total applied dose received by the receptor. In the Superfund program, EPA has traditionally focused on quantifying exposures to a receptor that are clearly site-related and has not included exposures from other sources such as commercially available household products or workplace exposures. Depending on the assumptions concerning other source contributions, apportionment among pathways and sources at a site may result in **more conservative** regulatory levels (e.g., levels that are below an HQ of 1). Depending on site conditions, this may be appropriate on a site-specific basis.

In contrast to apportionment, **fractionation** of risk may lead to **less conservative** regulatory levels because it assumes that some fraction of the contaminant does not reach the receptor due to partitioning into another medium. For example, if only one-fifth of the source is assumed to be available to the ground water pathway, and the remaining four-fifths is assumed to be released to air or remain in the soil, an SSL for the migration to ground water pathway could be set at five times the HQ of 1 due to the decrease in exposure (since only one-fifth of the possible contaminant is available to the pathway). However, the data collected to apply SSLs generally will not support the finite source models necessary for partitioning contaminants between pathways.

2.1.3 Acute Exposures. The exposure assumptions used to develop SSLs are representative of a chronic exposure scenario and do not account for situations where high-level exposures may lead to acute toxicity. For example, in some cases, children may ingest large amounts of soil (e.g., 3 to 5 grams) in a single event. This behavior, known as pica, may result in relatively high short-term exposures to contaminants in soils. Such exposures may be of concern for contaminants that primarily exhibit acute health effects. Review of clinical reports on contaminants addressed in this guidance suggests that acute effects of **cyanide** and **phenol** may be of concern in children exhibiting pica behavior. If soils containing cyanide and phenol are present at a site, the protectiveness of the chronic ingestion SSLs for these chemicals should be reconsidered.

Although the Soil Screening Guidance instructs site managers to consider the potential for acute exposures on a site-specific basis, there are two major impediments to developing **acute** SSLs. First, although data are available on chronic exposures (i.e., RfDs, RfCs, cancer slope factors), there is a paucity of data relating the potential for acute effects for most Superfund chemicals. Specifically, there is no scale to evaluate the severity of acute effects (e.g., eye irritation vs. dermatitis), no consensus on how to incorporate the body's recovery mechanisms following acute exposures, and no toxicity benchmarks to apply for short-term exposures (e.g., a 7-day RfD for a critical endpoint).

Table 2. SSL Chemicals with Noncarcinogenic Effects on Specific Target Organ/System

Target Organ/System	Effect
Kidney	
Acetone	Increased weight; nephrotoxicity
1,1-Dichloroethane	Kidney damage
Cadmium	Significant proteinuria
Chlorobenzene	Kidney effects
Di-*n*-octyl phthalate	Kidney effects
Endosulfan	Glomerulonephrosis
Ethylbenzene	Kidney toxicity
Fluoranthene	Nephropathy
Nitrobenzene	Renal and adrenal lesions
Pyrene	Kidney effects
Toluene	Changes in kidney weights
2,4,5-Trichlorophenol	Pathology
Vinyl acetate	Altered kidney weight
Liver	
Acenaphthene	Hepatotoxicity
Acetone	Increased weight
Butyl benzyl phthalate	Increased liver-to-body weight and liver-to-brain weight ratios
Chlorobenzene	Histopathology
Di-*n*-octyl phthalate	Increased weight; increased SGOT and SGPT activity
Endrin	Mild histological lesions in liver
Flouranthene	Increased liver weight
Nitrobenzene	Lesions
Styrene	Liver effects
Toluene	Changes in liver weights
2,4,5-Trichlorophenol	Pathology
Central Nervous System	
Butanol	Hypoactivity and ataxia
Cyanide (amenable)	Weight loss, myelin degeneration
2,4 Dimethylphenol	Prostatration and ataxia
Endrin	Occasional convulsions
2-Methylphenol	Neurotoxicity
Mercury	Hand tremor, memory disturbances
Styrene	Neurotoxicity
Xylenes	Hyperactivity
Adrenal Gland	
Nitrobenzene	Adrenal lesions
1,2,4-Trichlorobenzene	Increased adrenal weights; vacuolization in cortex

Table 2: (continued)

Target Organ/System	Effect
Circulatory System	
Antimony	Altered blood chemistry and myocardial effects
Barium	Increased blood pressure
trans-1,2-Dichloroethene	Increased alkaline phosphatase level
cis-1,2-Dichloroethylene	Decreased hematocrit and hemoglobin
2,4-Dimethylphenol	Altered blood chemistry
Fluoranthene	Hematologic changes
Fluorene	Decreased RBC and hemoglobin
Nitrobenzene	Hematologic changes
Styrene	Red blood cell effects
Zinc	Decrease in erythrocyte superoxide dismutase (ESOD)
Reproductive System	
Barium	Fetotoxicity
Carbon disulfide	Fetal toxicity and malformations
2-Chlorophenol	Reproductive effects
Methoxychlor	Excessive loss of litters
Phenol	Reduced fetal body weight in rats
Respiratory System	
1,2-Dichloropropane	Hyperplasia of the nasal mucosa
Hexachlorocyclopentadiene	Squamous metaplasia
Methyl bromide	Lesions on the olfactory epithelium of the nasal cavity
Vinyl acetate	Nasal epithelial lesions
Gastrointestinal System	
Hexachlorocyclopentadiene	Stomach lesions
Methyl bromide	Epithelial hyperplasia of the forestomach
Immune System	
2,4-Dichlorophenol	Altered immune function
p-Chloroaniline	Nonneoplastic lesions of splenic capsule

Source: U.S. EPA, 1995b, U.S. EPA, 1995d.

Second, the inclusion of acute SSLs would require the development of acute exposure scenarios that would be acceptable and applicable nationally. Simply put, the methodology and data necessary to address acute exposures in a standard manner analogous to that for chronic exposures have not been developed.

2.1.4 Route-to-Route Extrapolation. For a number of the contaminants commonly found at Superfund sites, inhalation benchmarks for toxicity are not available from IRIS or HEAST (see Table 1). Given that many of these chemicals exhibit systemic toxicity, EPA recognizes that the lack of such benchmarks could result in an underestimation of risk from contaminants in soil through the inhalation pathway. As pointed out by commenters to the December 1994 draft Soil Screening Guidance, ingestion SSLs tend to be higher than inhalation SSLs for most volatile chemicals with both inhalation and ingestion benchmarks. This suggests that ingestion SSLs may not be adequately protective for inhalation exposure to chemicals without inhalation benchmarks.

However, with the exception of vinyl chloride (which is gaseous at ambient temperatures), migration to ground water SSLs are significantly lower than inhalation SSLs for volatile organic chemicals (see the generic SSLs presented in Appendix A). Thus, at sites where ground water is of concern, migration to ground water SSLs generally will be protective from the standpoint of inhalation risk. However, if the ground water pathway is not of concern at a site, the use of SSLs for soil ingestion may not be adequately protective for the inhalation pathway.

To address this concern, OERR evaluated potential approaches for deriving inhalation benchmarks using route-to-route extrapolation from oral benchmarks (e.g., RfC_{inh} from RfD_{oral}). EPA evaluated a number of issues concerning route-to-route extrapolation, including: the potential reactivity of airborne toxicants (e.g., portal-of-entry effects), the pharmacokinetic behavior of toxicants for different routes of exposure (e.g., absorption by the gut versus absorption by the lung), and the significance of physicochemical properties in determining dose (e.g., vapor pressure, solubility). During this process, OERR consulted with staff in the EPA Office of Research and Development (ORD) to identify the most appropriate techniques for route-to-route extrapolation. Appendix B describes this analysis and its results.

As part of this analysis, inhalation benchmarks were derived using simple route-to-route extrapolation for 50 contaminants lacking inhalation benchmarks. A review of SSLs calculated from these extrapolated benchmarks indicated that for 36 of the 50 contaminants, inhalation SSLs exceed the soil saturation concentration (C_{sat}), often by several orders of magnitude. Because maximum volatile emissions occur at C_{sat} (see Section 2.4.4), these 36 contaminants are not likely to pose significant risks through the inhalation pathway at any soil concentration and the lack of inhalation benchmarks is not likely to underestimate risks. All of the 14 remaining contaminants with extrapolated inhalation SSLs below C_{sat} have inhalation SSLs above generic SSLs for the migration to ground water pathway (dilution attenuation factor [DAF] of 20). This suggests that migration to ground water SSLs will be adequately protective of volatile inhalation risks at sites where ground water is of concern.

At sites where ground water is not of concern (e.g., where ground water beneath or adjacent to the site is not a potential source of drinking water), the Appendix B analysis suggests that for certain contaminants, ingestion SSLs may not be protective of inhalation risks for contaminants lacking inhalation benchmarks. The analysis indicates that the extrapolated inhalation SSL values are below SSL values based on direct ingestion for the following chemicals: acetone, bromodichloromethane, chlorodibromomethane, *cis*-1,2-dichloroethylene, and *trans*-1,2-dichloroethylene. This supports the **possibility** that the SSLs based on direct ingestion for the listed chemicals may not be adequately protective of inhalation exposures. However, because this analysis is based on simplified route-to-route extrapolation methods, a more rigorous evaluation of route-to-route extrapolation methods may be warranted, especially at sites where ground water is not of concern.

Based on these results, EPA reached the following conclusions regarding the route-to-route extrapolation of inhalation benchmarks for the development of inhalation SSLs. First, it is reasonable to assume that, for some volatile contaminants, the lack of inhalation benchmarks may underestimate risks due to inhalation of volatile contaminants at a site. However, the analysis in Appendix B suggests that this issue is only of concern for sites where the exposure potential for the inhalation pathway approaches that for ingestion of ground water or at sites where the migration to ground water pathway is not of concern.

Second, the **extrapolated** inhalation SSL values are not intended to be used as generic SSLs for site investigations; the **extrapolated** inhalation SSLs are useful in determining the potential for inhalation risks but should not be misused as SSLs. The extrapolated inhalation benchmarks, used to calculate extrapolated inhalation SSLs, simply provide an estimate of the air concentration ($\mu g/m^3$)

required to produce an inhaled dose equivalent to the dose received via oral administration, and lack the scientific rigor required by EPA for route-to-route extrapolation. Route-to-route extrapolation methods must account for a relationship between physicochemical properties, absorption and distribution of toxicants, the significance of portal-of-entry effects, and the potential differences in metabolic pathways associated with the intensity and duration of inhalation exposures. However, methods required to develop sufficiently rigorous inhalation benchmarks have only recently been developed by the ORD. EPA's ORD has made available a guidance document that addresses many of the issues critical to the development of inhalation benchmarks. The document, entitled *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry* (U.S. EPA, 1994d), presents methods for applying inhalation dosimetry to derive inhalation reference concentrations and represents the current state-of-the-science at EPA with respect to inhalation benchmark development. The fundamentals of inhalation dosimetry are presented with respect to the toxicokinetic behavior of contaminants and the physicochemical properties of chemical contaminants.

Thus, at sites where the migration to ground water pathway is not of concern and a site manager determines that the inhalation pathway may be significant for contaminants lacking inhalation benchmarks, route-to-route extrapolation may be performed using EPA-approved methods on a case-by-case basis. Chemical-specific route-to-route extrapolations should be accompanied by a complete discussion of the data, underlying assumptions, and uncertainties identified in the extrapolation process. Extrapolation methods should be consistent with the EPA guidance presented in *Methods for Derivation of Inhalation Reference Concentrations and Applications of Inhalation Dosimetry* (U.S. EPA, 1994d). If a route-to-route extrapolation is found not to be appropriate based on the ORD guidance, the information on extrapolated SSLs may be included as part of the uncertainty analysis of the baseline risk assessment for the site.

2.2 Direct Ingestion

Calculation of SSLs for direct ingestion of soil is based on the methodology presented for residential land use in RAGS HHEM, Part B (U.S. EPA, 1991b). Briefly, this methodology backcalculates a soil concentration level from a target risk (for carcinogens) or hazard quotient (for noncarcinogens). A number of studies have shown that inadvertent ingestion of soil is common among children 6 years old and younger (Calabrese et al., 1989; Davis et al., 1990; Van Wijnen et al., 1990). Therefore, the approach uses an age-adjusted soil ingestion factor that takes into account the difference in daily soil ingestion rates, body weights, and exposure duration for children from 1 to 6 years old and others from 7 to 31 years old. The higher intake rate of soil by children and their lower body weights lead to a lower, or more conservative, risk-based concentration compared to an adult-only assumption. RAGS HHEM, Part B uses this age-adjusted approach for both noncarcinogens and carcinogens.

For noncarcinogens, the definition of an RfD has led to debates concerning the comparison of less-than-lifetime estimates of exposure to the RfD. Specifically, it is often asked whether the comparison of a 6-year exposure, estimated for children via soil ingestion, to the chronic RfD is unnecessarily conservative.

In their analysis of the issue, the SAB indicates that, for most chemicals, the approach of combining the higher 6-year exposure for children with chronic toxicity criteria is overly protective (U.S. EPA, 1993e). However, they noted that there are instances when the chronic RfD may be based on endpoints of toxicity that are specific to children (e.g., fluoride and nitrates) or when the dose-response curve is steep (i.e., the dosage difference between the no-observed-adverse-effects level [NOAEL] and an adverse effects level is small). Thus, for the purposes of screening, OERR opted to base the generic SSLs for noncarcinogenic contaminants on the more conservative “childhood only” exposure (Equation 1). The issue of whether to maintain this more conservative approach throughout the baseline risk assessment and establishing remediation goals will depend on how the toxicology of the chemical relates to the issues raised by the SAB.

Screening Level Equation for Ingestion of Noncarcinogenic Contaminants in Residential Soil

(Source: RAGS HHEM, Part B; U.S. EPA, 1991b)

$$\text{Screening Level (mg/kg)} = \frac{\text{THQ} \times \text{BW} \times \text{AT} \times 365\ \text{d/yr}}{1/\text{RfD}_o \times 10^{-6}\ \text{kg/mg} \times \text{EF} \times \text{ED} \times \text{IR}} \quad \textbf{(1)}$$

Parameter/Definition (units)	Default
THQ/target hazard quotient (unitless)	1
BW/body weight (kg)	15
AT/averaging time (yr)	6[a]
RfD_o /oral reference dose (mg/kg-d)	chemical-specific
EF/exposure frequency (d/yr)	350
ED/exposure duration (yr)	6
IR/soil ingestion rate (mg/d)	200

[a] For noncarcinogens, averaging time is equal to exposure duration. Unlike RAGS HHEM, Part B, SSLs are calculated only for 6-year childhood exposure.

For carcinogens, both the magnitude and duration of exposure are important. Duration is critical because the toxicity criteria are based on "lifetime average daily dose." Therefore, the total dose received, whether it be over 5 years or 50 years, is averaged over a lifetime of 70 years. To be protective of exposures to carcinogens in the residential setting, RAGS HHEM, Part B (U.S. EPA, 1991b) and EPA focus on exposures to individuals who may live in the same residence for a "high-end" period of time (e.g., 30 years). As mentioned above, exposure to soil is higher during childhood and decreases with age. Thus, Equation 2 uses the RAGS HHEM, Part B time-weighted average soil ingestion rate for children and adults; the derivation of this factor is shown in Equation 3.

Screening Level Equation for Ingestion of Carcinogenic Contaminants in Residential Soil

(Source: RAGS HHEM, Part B; U.S. EPA, 1991b)

$$\text{Screening Level (mg/kg)} = \frac{\text{TR} \times \text{AT} \times 365\ \text{d/yr}}{\text{SF}_o \times 10^{-6}\ \text{kg/mg} \times \text{EF} \times \text{IF}_{\text{soil/adj}}} \quad \textbf{(2)}$$

Parameter/Definition (units)	Default
TR/target cancer risk (unitless)	10^{-6}
AT/averaging time (yr)	70
SF_o /oral slope factor $(mg/kg\text{-}d)^{-1}$	chemical-specific
EF/exposure frequency (d/yr)	350
$IF_{soil/adj}$ /age-adjusted soil ingestion factor (mg-yr/kg-d)	114

Equation for Age-Adjusted Soil Ingestion Factor, $IF_{soil/adj}$

$$\begin{array}{c} IF_{soil/adj} \\ (mg\text{-}yr/kg\text{-}d) \end{array} = \frac{IR_{soil/age1\text{-}6} \times ED_{age1\text{-}6}}{BW_{age1\text{-}6}} + \frac{IR_{soil/age7\text{-}31} \times ED_{age7\text{-}31}}{BW_{age7\text{-}31}} \tag{3}$$

Parameter/Definition (units)	Default
$IF_{soil/adj}$ /age-adjusted soil ingestion factor (mg-yr/kg-d)	114
$IR_{soil/age1\text{-}6}$ /ingestion rate of soil age 1-6 (mg/d)	200
$ED_{age1\text{-}6}$ /exposure duration during ages 1-6 (yr)	6
$IR_{soil/age7\text{-}31}$ /ingestion rate of soil age 7-31 (mg/d)	100
$ED_{age7\text{-}31}$ /exposure duration during ages 7-31 (yr)	24
$BW_{age1\text{-}6}$ /average body weight from ages 1-6 (kg)	15
$BW_{age7\text{-}31}$ /average body weight from ages 7-31 (kg)	70

Source: RAGS HHEM, Part B (U.S. EPA, 1991b).

Because of the impracticability of developing site-specific input parameters (e.g., soil ingestion rates, chemical-specific bioavailability) for direct soil ingestion, SSLs are calculated using the defaults listed in Equations 1, 2, and 3. Appendix A lists these generic SSLs for direct ingestion of soil.

2.3 Dermal Absorption

Incorporation of dermal exposures into the Soil Screening Guidance is limited by the amount of data available to quantify dermal absorption from soil for specific chemicals. EPA's ORD evaluated the available data on absorption of chemicals from soil in the document *Dermal Exposure Assessment: Principles and Applications* (U.S. EPA, 1992b). This document also presents calculations comparing the potential dose of a chemical in soil from oral routes with that from dermal routes of exposure.

These calculations suggest that, assuming 100 percent absorption of a chemical via ingestion, absorption via the dermal route must be greater than 10 percent to equal or exceed the ingestion exposure. Of the 110 compounds evaluated, available data are adequate to show greater than 10 percent dermal absorption only for pentachlorophenol (Wester et al., 1993). Therefore, the ingestion SSL for pentachlorophenol is adjusted to account for this additional exposure (i.e., the ingestion SSL has been divided in half to account for increased exposure via the dermal route). Limited data suggest that dermal absorption of other semivolatile organic chemicals (e.g., benzo(*a*)pyrene) from soil may exceed 10 percent (Wester et al., 1990) but EPA believes that further investigation is needed. As adequate dermal absorption data are developed for such chemicals the ingestion SSLs may need to be adjusted. EPA will provide updates on this issue as appropriate.

2.4 Inhalation of Volatiles and Fugitive Dusts

EPA toxicity data indicate that risks from exposure to some chemicals via inhalation far outweigh the risks via ingestion; therefore, the SSLs have been designed to address this pathway as well. The models and assumptions used to calculate SSLs for inhalation of volatiles are updates of risk assessment methods presented in RAGS HHEM, Part B (U.S. EPA, 1991b). RAGS HHEM, Part B evaluated the contribution to risk from the inhalation and ingestion pathways simultaneously. Because toxicity criteria for oral exposures are presented as administered doses (in mg/kg-d) and criteria for inhalation exposures are presented as concentrations in air (in µg/m^3), conversion of air concentrations was required to estimate an administered dose comparable to the oral route. However, EPA's ORD now believes that, due to portal-of-entry effects and differences in absorption in the gut versus the lungs, the conversion from concentration in air to internal dose is not always appropriate and suggests evaluating these exposure routes separately.

The models and assumptions used to calculate SSLs for the inhalation pathway are presented in Equations 4 through 12, along with the default parameter values used to calculate the generic SSLs presented in Appendix A. Particular attention is given to the volatilization factor (VF), saturation limit (C_{sat}), and the dispersion portion of the VF and particulate emission factor (PEF) equations, all of which have been revised since originally presented in RAGS HHEM, Part B. The available chemical-specific human health benchmarks used in these equations are presented in Section 2.1. Part 5 presents the chemical properties required by these equations, along with the rationale for their selection and development.

2.4.1 Screening Level Equations for Direct Inhalation. Equations 4 and 5 are used to calculate SSLs for the inhalation of carcinogenic and noncarcinogenic contaminants, respectively. Each equation addresses volatile compounds and fugitive dusts separately for developing screening levels based on inhalation risk for subsurface soils and surface soils.

Separate VF-based and PEF-based equations were developed because the SSL sampling strategy addresses surface and subsurface soils separately. Inhalation risk from fugitive dusts results from particle entrainment from the soil surface; thus contaminant concentrations in the surface soil horizon (e.g., the top 2 centimeters) are of primary concern for this pathway. The entire column of contaminated soil can contribute to volatile emissions at a site. However, the top 2 centimeters are likely to be depleted of volatile contaminants at most sites. Thus, contaminant concentrations in subsurface soils, which are measured using core samples, are of primary concern for quantifying the risk from volatile emissions.

Screening Level Equation for Inhalation of Carcinogenic Contaminants in Residential Soil

$$\text{Volatile Screening Level (mg/kg)} = \frac{\text{TR} \times \text{AT} \times 365\ \text{d/yr}}{\text{URF} \times 1{,}000\ \mu\text{g/mg} \times \text{EF} \times \text{ED} \times \left[\frac{1}{\text{VF}}\right]} \qquad \textbf{(4)}$$

$$\text{Particulate Screening Level (mg/kg)} = \frac{\text{TR} \times \text{AT} \times 365\ \text{d/yr}}{\text{URF} \times 1{,}000\ \mu\text{g/mg} \times \text{EF} \times \text{ED} \times \left[\frac{1}{\text{PEF}}\right]}$$

Parameter/Definition (units)	Default
TR/target cancer risk (unitless)	10^{-6}
AT/averaging time (yr)	70
URF/inhalation unit risk factor ($\mu g/m^3)^{-1}$	chemical-specific
EF/exposure frequency (d/yr)	350
ED/exposure duration (yr)	30
VF/soil-to-air volatilization factor (m^3/kg)	chemical-specific
PEF/particulate emission factor (m^3/kg)	1.32×10^9

Source: RAGS HHEM, Part B (U.S. EPA, 1991b).

Screening Level Equation for Inhalation of Noncarcinogenic Contaminants in Residential Soil

$$\text{Volatile Screening Level (mg/kg)} = \frac{\text{THQ} \times \text{AT} \times 365\ \text{d/yr}}{\text{EF} \times \text{ED} \times \left(\frac{1}{\text{RfC}} \times \frac{1}{\text{VF}}\right)} \qquad \textbf{(5)}$$

$$\text{Particulate Screening Level (mg/kg)} = \frac{\text{THQ} \times \text{AT} \times 365\ \text{d/yr}}{\text{EF} \times \text{ED} \times \left(\frac{1}{\text{RfC}} \times \frac{1}{\text{PEF}}\right)}$$

Parameter/Definition (units)	Default
THQ/target hazard quotient (unitless)	1
AT/averaging time (yr)	30
EF/exposure frequency (d/yr)	350
ED/exposure duration (yr)	30
RfC/inhalation reference concentration (mg/m^3)	chemical-specific
VF/soil-to-air volatilization factor (m^3/kg)	chemical-specific
PEF/particulate emission factor (m^3/kg) (Equation 10)	1.32×10^9

Source: RAGS HHEM, Part B (U.S. EPA, 1991b).

To calculate inhalation SSLs, the volatilization factor and particulate emission factor must be calculated. The derivations of VF and PEF have been updated since RAGS HHEM, Part B was published and are discussed fully in Sections 2.4.2 and 2.4.5, respectively. The VF and PEF equations can be broken into two separate models: models to estimate the emissions of volatiles and dusts, and a dispersion model (reduced to the term Q/C) that simulates the dispersion of contaminants in the atmosphere.

2.4.2 Volatilization Factor. The soil-to-air VF is used to define the relationship between the concentration of the contaminant in soil and the flux of the volatilized contaminant to air. VF is calculated from Equation 6 using chemical-specific properties (see Part 5) and either site-measured or default values for soil moisture, dry bulk density, and fraction of organic carbon in soil. The User's Guide (U.S. EPA, 1996) describes how to develop site measured values for these parameters.

Derivation of Volatilization Factor

(6)

$$\mathrm{VF}\,(\mathrm{m}^3/\mathrm{kg}) = \mathrm{Q/C} \times \frac{(3.14 \times D_A \times T)^{1/2}}{(2 \times \rho_b \times D_A)} \times 10^{-4}(\mathrm{m}^2/\mathrm{cm}^2)$$

where

$$D_A = \frac{\left[(\theta_a^{10/3} D_i H' + \theta_w^{10/3} D_w)/n^2\right]}{\rho_b K_d + \theta_w + \theta_a H'}$$

Parameter/Definition (units)	Default	Source
VF/volatilization factor (m^3/kg)	–	–
D_A /apparent diffusivity (cm^2/s)	–	–
Q/C/inverse of the mean conc. at center of square source (g/m^2-s per kg/m^3)	68.81	Table 3 (for 0.5-acre source in Los Angeles, CA)
T/exposure interval (s)	9.5×10^8	U.S. EPA (1991b)
ρ_b/dry soil bulk density (g/cm^3)	1.5	U.S. EPA (1991b)
θ_a /air-filled soil porosity (L_{air}/L_{soil})	0.28	n - θ_w
n/total soil porosity (L_{pore}/L_{soil})	0.43	1 - (ρ_b/ρ_s)
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.15	EQ, 1994
ρ_s /soil particle density (g/cm^3)	2.65	U.S. EPA (1991b)
D_i /diffusivity in air (cm^2/s)	chemical-specific	see Part 5
H′/dimensionless Henry's law constant	chemical-specific	see Part 5
D_w /diffusivity in water (cm^2/s)	chemical-specific	see Part 5
K_d /soil-water partition coefficient (cm^3/g) = K_{oc} f_{oc}	chemical-specific	see Part 5
K_{oc} /soil organic carbon-water partition coefficient (cm^3/g)	chemical-specific	see Part 5
f_{oc}/organic carbon content of soil (g/g)	0.006 (0.6%)	Carsel et al. (1988)

The VF equation presented in Equation 6 is based on the volatilization model developed by Jury et al. (1984) for infinite sources and is theoretically consistent with the Jury et al. (1990) finite source volatilization model (see Section 3.1). This equation represents a change in the fundamental volatilization model used to derive the VF equation used in RAGS HHEM, Part B and in the December 1994 draft Soil Screening Guidance (U.S. EPA, 1994h).

The VF equation presented in RAGS HHEM, Part B is based on the volatilization model developed by Hwang and Falco (1986) for dry soils. During the reevaluation of RAGS HHEM, Part B, EPA sponsored a study (see the December 1994 draft Technical Background Document, U.S. EPA, 1994i) to validate the VF equation by comparing the modeled results with data from (1) a bench-scale pesticide study (Farmer and Letey, 1974) and (2) a pilot-scale study measuring the rate of loss of benzene, toluene, xylenes, and ethylbenzene from soils using an isolation flux chamber (Radian, 1989). The results of the study verified the need to modify the VF equation in Part B to take into account the decrease in the rate of flux due to the effect of soil moisture content on effective diffusivity (D_{ei}).

In the December 1994 version of this background document (U.S. EPA, 1994i), the Hwang and Falco model was modified to account for the influence of soil moisture on the effective diffusivity using the Millington and Quirk (1961) equation. However, inconsistencies were discovered in the modified Hwang and Falco equations. Additionally, even a correctly modified Hwang and Falco model does not consider the influence of the liquid phase on the local equilibrium partitioning. Consequently, EPA evaluated the Jury model for its ability to predict emissions measured in pilot-scale volatilization studies (Appendix C; EQ, 1995). The infinite source Jury model emission rate predictions were consistently within a factor of 2 of the emission rates measured in the pilot-scale volatilization studies. Because the Jury model predicts well the available measured soil contaminant volatilization rates, eliminates the inconsistencies of the modified Hwang and Falco model, and considers the influence of the liquid phase on the local equilibrium partitioning, it was selected to replace the modified Hwang and Falco model for the derivation of the VF equation.

Defaults. Other than initial soil concentration, air-filled soil porosity is the most significant soil parameter affecting the final steady-state flux of volatile contaminants from soil (U.S. EPA, 1980). In other words, the higher the air-filled soil porosity, the greater the emission flux of volatile constituents. Air-filled soil porosity is calculated as:

$$\theta_a = n - \theta_w \qquad \textbf{(7)}$$

where

θ_a = air-filled soil porosity (L_{air}/L_{soil})
n = total soil porosity (L_{pore}/L_{soil})
θ_w = water-filled soil porosity (L_{water}/L_{soil})

and

$$n = 1 - (\rho_b/\rho_s) \qquad \textbf{(8)}$$

where

ρ_b = dry soil bulk density (g/cm^3)
ρ_s = soil particle density (g/cm^3).

Of these parameters, water-filled soil porosity (θ_w) has the most significant effect on air-filled soil porosity and hence volatile contaminant emissions. Sensitivity analyses have shown that soil bulk density (ρ_b) has too limited a range for surface soils (generally between 1.3 and 1.7 g/cm^3) to affect results with nearly the significance of soil moisture conditions. Therefore, a default bulk density of 1.50 g/cm^3, the mode of the range given for U.S. soils in the *Superfund Exposure Assessment Manual* (U.S. EPA, 1988), was chosen to calculate generic SSLs. This value is also consistent with the mean porosity (0.43) for loam soil presented in Carsel and Parrish (1988).

The default value of θ_w (0.15) corresponds to an average annual soil water content of 10 weight percent. This value was chosen as a conservative compromise between that required to achieve a monomolecular layer of water on soil particles (approximately 2 to 5 weight percent) and that required to reduce the air-filled porosity to zero (approximately 29 weight percent). In this manner, nonpolar or weakly polar contaminants are desorbed readily from the soil organic carbon as water competes for sorption sites. At the same time, a soil moisture content of 10 percent yields a relatively conservative air-filled porosity (0.28 or 28 percent by volume). A water-filled soil porosity (θ_w) of 0.15 lies about halfway between the mean wilting point (0.09) and mean field capacity (0.20) reported for Class B soils by Carsel et al. (1988). Class B soils are soils with moderate hydrologic characteristics whose average characteristics are well represented by a loam soil type.

The default value of ρ_s (2.65 g/cm^3) was taken from U.S. EPA (1988) as the particle density for most soil mineral material. The default value for f_{oc} (0.006 or 0.6 percent) is the mean value for the top 0.3 m of Class B soils from Carsel et al. (1988).

2.4.3 Dispersion Model. The box model in RAGS HHEM, Part B has been replaced with a Q/C term derived from a modeling exercise using meteorologic data from 29 locations across the United States.

The dispersion model used in the Part B guidance is based on the assumption that emissions into a hypothetical box will be distributed uniformly throughout the box. To arrive at the volume within the box, it is necessary to assign values to the length, width, and height of the box. The length (LS) was the length of a side of a contaminated site with a default value of 45 m; the width was based on the windspeed in the mixing zone (V) with a default value of 2.25 m (based on a windspeed of 2.25 m/s); and the height was the diffusion height (DH) with a default value of 2 m.

However, the assumptions and mathematical treatment of dispersion used in the box model may not be applicable to a broad range of site types and meteorology and do not utilize state-of-the-art techniques developed for regulatory dispersion modeling. EPA was very concerned about the defensibility of the box model and sought a more defensible dispersion model that could be used as a replacement to the Part B guidance and had the following characteristics:

- Dispersion modeling from a ground-level area source
- Onsite receptor
- A long-term/annual average exposure point concentration
- Algorithms for calculating the exposure point concentration for area sources of different sizes and shapes.

To identify such a model, EPA held discussions with the EPA Office of Air Quality Planning and Standards (OAQPS) concerning recent efforts to develop a new algorithm for estimating ambient air concentrations from low or ground-level, nonbuoyant sources of emissions. The new algorithm is incorporated into the Industrial Source Complex Model (ISC2) platform in both a short-term mode (AREA-ST) and a long-term mode (AREA-LT). Both models employ a double numerical integration over the source in the upwind and crosswind directions. Wind tunnel tests have shown that the new algorithm performs well with onsite and near-field receptors. In addition, subdivision of the source is not required for these receptors.

Because the new algorithm provides better concentration estimates for onsite and for near-field receptors, a revised dispersion analysis was performed for both volatile and particulate matter contaminants (Appendix D; EQ, 1994). The AREA-ST model was run for 0.5-acre and 30-acre square sources with a full year of meteorologic data for 29 U.S locations selected to be representative of the national range of meteorologic conditions (EQ, 1993). Additional modeling runs were conducted to address a range of square area sources from 0.5 to 30 acres in size (Table 3). The Q/C values in Table 3 for 0.5- and 30-acre sources differ slightly from the values in Appendix D due to differences in rounding conventions used in the final model runs.

To calculate site-specific SSLs, select a Q/C value from Table 3 that best represents a site's size and meteorologic condition.

To develop a reasonably conservative default Q/C for calculating generic SSLs, a default site (Los Angeles, CA) was chosen that best approximated the 90th percentile of the 29 normalized concentrations (kg/m^3 per g/m^2-s). The inverse of this concentration results in a default VF Q/C value of 68.81 g/m^2-s per kg/m^3 for a 0.5-acre site.

Table 3. Q/C Values by Source Area, City, and Climatic Zone

	Q/C (g/m^2-s per kg/m^3)					
	0.5 Acre	1 Acre	2 Acre	5 Acre	10 Acre	30 Acre
Zone I						
Seattle	82.72	72.62	64.38	55.66	50.09	42.86
Salem	73.44	64.42	57.09	49.33	44.37	37.94
Zone II						
Fresno	62.00	54.37	48.16	41.57	37.36	31.90
Los Angeles	68.81	60.24	53.30	45.93	41.24	35.15
San Francisco	89.51	78.51	69.55	60.03	53.95	46.03
Zone III						
Las Vegas	95.55	83.87	74.38	64.32	57.90	49.56
Phoenix	64.04	56.07	49.59	42.72	38.35	32.68
Albuquerque	84.18	73.82	65.40	56.47	50.77	43.37
Zone IV						
Boise	69.41	60.88	53.94	46.57	41.87	35.75
Winnemucca	69.23	60.67	53.72	46.35	41.65	35.55
Salt Lake City	78.09	68.47	60.66	52.37	47.08	40.20
Casper	100.13	87.87	77.91	67.34	60.59	51.80
Denver	75.59	66.27	58.68	50.64	45.52	38.87
Zone V						
Bismark	83.39	73.07	64.71	55.82	50.16	42.79
Minneapolis	90.80	79.68	70.64	61.03	54.90	46.92
Lincoln	81.64	71.47	63.22	54.47	48.89	41.65
Zone VI						
Little Rock	73.63	64.51	57.10	49.23	44.19	37.64
Houston	79.25	69.47	61.53	53.11	47.74	40.76
Atlanta	77.08	67.56	59.83	51.62	46.37	39.54
Charleston	74.89	65.65	58.13	50.17	45.08	38.48
Raleigh-Durham	77.26	67.75	60.01	51.78	46.51	39.64
Zone VII						
Chicago	97.78	85.81	76.08	65.75	59.16	50.60
Cleveland	83.22	73.06	64.78	55.99	50.38	43.08
Huntington	53.89	47.24	41.83	36.10	32.43	27.67
Harrisburg	81.90	71.87	63.72	55.07	49.56	42.40
Zone VIII						
Portland	74.23	65.01	57.52	49.57	44.49	37.88
Hartford	71.35	62.55	55.40	47.83	43.00	36.73
Philadelphia	90.24	79.14	70.14	60.59	54.50	46.59
Zone IX						
Miami	85.61	74.97	66.33	57.17	51.33	43.74

2.4.4 Soil Saturation Limit. The soil saturation concentration (C_{sat}) corresponds to the contaminant concentration in soil at which the absorptive limits of the soil particles, the solubility limits of the soil pore water, and saturation of soil pore air have been reached. Above this concentration, the soil contaminant may be present in free phase, i.e., nonaqueous phase liquids (NAPLs) for contaminants that are liquid at ambient soil temperatures and pure solid phases for compounds that are solid at ambient soil temperatures.

Derivation of the Soil Saturation Limit

$$C_{sat} = \frac{S}{\rho_b} \left(K_d \, \rho_b + \theta_w + H' \, \theta_a \right) \tag{9}$$

Parameter/Definition (units)	Default	Source
C_{sat}/soil saturation concentration (mg/kg)	–	
S/solubility in water (mg/L-water)	chemical-specific	see Part 5
ρ_b/dry soil bulk density (kg/L)	1.5	U.S. EPA, 1991b
K_d/soil-water partition coefficient (L/kg)	$K_{oc} \times f_{oc}$ (organics)	
K_{oc}/soil organic carbon/water partition coefficient (L/kg)	chemical-specific	see Part 5
f_{oc}/fraction organic carbon of soil (g/g)	0.006 (0.6%)	Carsel et al., 1988
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.15	EQ, 1994
H′/dimensionless Henry's law constant	H x 41, where 41 is a conversion factor	U.S. EPA, 1991b
H/Henry's law constant (atm-m^3/mol)	chemical-specific	see Part 5
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.28	$n - \theta_w$
n/total soil porosity (L_{pore}/L_{soil})	0.43	$1 - \rho_b/\rho_s$
ρ_s/soil particle density (kg/L)	2.65	U.S. EPA, 1991b

Equation 9 is used to calculate C_{sat} for each site contaminant. As an update to RAGS HHEM, Part B, this equation takes into account the amount of contaminant that is in the vapor phase in the pore spaces of the soil in addition to the amount dissolved in the soil's pore water and sorbed to soil particles.

Chemical-specific C_{sat} concentrations must be compared with each volatile inhalation SSL because a basic principle of the SSL volatilization model (Henry's law) is not applicable when free-phase contaminants are present (i.e., the model cannot predict an accurate VF or SSL above C_{sat}). Thus, the VF-based inhalation SSLs are applicable only if the soil concentration is at or below C_{sat}. When calculating volatile inhalation SSLs, C_{sat} values also should be calculated using the same site-specific soil characteristics used to calculate SSLs (i.e., bulk density, average water content, and organic carbon content).

At C_{sat} the emission flux from soil to air for a chemical reaches a plateau. Volatile emissions will not increase above this level no matter how much more chemical is added to the soil. Table 3-A shows that for compounds with generic volatile inhalation SSLs greater than C_{sat}, the risks at C_{sat} are significantly below the screening risk of 1×10^{-6} and an HQ of 1. Since C_{sat} corresponds to maximum volatile emissions, the inhalation route is not likely to be of concern for those chemicals with SSLs exceeding C_{sat} concentrations.

Table 3-A. Risk Levels Calculated at C_{sat} for Contaminants that have SSL_{inh} Values Greater than C_{sat}

Chemical name	URF (µg/m^3)$^{-1}$	RfC (mg/m^3)	VF (m^3/kg)	C_{sat} (mg/kg)	Carcinogenic Risk	Non-Carcinogenic Risk
DDT	9.7E-05	---	3.0E+07	4.0E+02	5.2E-07	---
1,2-Dichlorobenzene	---	2.0E-01	1.5E+04	6.0E+02	---	0.2
1,4-Dichlorobenzene	---	8.0E-01	1.3E+04	2.8E+02	---	0.03
Ethylbenzene	---	1.0E+00	5.4E+03	4.0E+02	---	0.07
β-HCH (β-BHC)	5.3E-04	---	1.3E+06	2.0E+00	3.4E-07	---
Styrene	---	1.0E+00	1.3E+04	1.5E+03	---	0.1
Toluene	---	4.0E-01	4.0E+03	6.5E+02	---	0.4
1,2,4-Trichlorobenzene	---	2.0E-01	4.3E+04	3.2E+03	---	0.4
1,1,1-Trichloroethane	---	1.0E+00	2.2E-03	1.2E+03	---	0.5

Table 4 provides the physical state (i.e. liquid or solid) for various compounds at ambient soil temperature. When the inhalation SSL exceeds C_{sat} for liquid compounds, the SSL is set at C_{sat}. This is because, for compounds that are liquid at ambient soil temperature, concentrations above C_{sat} indicate a potential for free liquid phase contamination to be present, and the possible presence of NAPLs. EPA believes that further investigation is warranted when free nonaqueous phase liquids may be present in soils at a site.

Table 4. Physical State of Organic SSL Chemicals

Compounds liquid at soil temperatures			Compounds solid at soil temperatures		
CAS No.	**Chemical**	**Melting Point (˚C)**	**CAS No.**	**Chemical**	**Melting Point (˚C)**
67-64-1	Acetone	-94.8	83-32-9	Acenaphthene	93.4
71-43-2	Benzene	5.5	309-00-2	Aldrin	104
117-81-7	Bis(2-ethylhexyl)phthalate	-55	120-12-7	Anthracene	215
111-44-4	Bis(2-chloroethyl)ether	-51.9	56-55-3	Benz(*a*)anthracene	84
75-27-4	Bromodichloromethane	-57	50-32-8	Benzo(*a*)pyrene	176.5
75-25-2	Bromoform	8	205-99-2	Benzo(*b*)fluoranthene	168
71-36-3	Butanol	-89.8	207-08-9	Benzo(*k*)fluoranthene	217
85-68-7	Butyl benzyl phthalate	-35	65-85-0	Benzoic acid	122.4
75-15-0	Carbon disulfide	-115	86-74-8	Carbazole	246.2
56-23-5	Carbon tetrachloride	-23	57-74-9	Chlordane	106
108-90-7	Chlorobenzene	-45.2	106-47-8	*p*-Chloroaniline	72.5
124-48-1	Chlorodibromomethane	-20	218-01-9	Chrysene	258.2
67-66-3	Chloroform	-63.6	72-54-8	DDD	109.5

Table 4. (continued)

Compounds liquid at soil temperatures			Compounds solid at soil temperatures		
CAS No.	Chemical	Melting Point (˚C)	CAS No.	Chemical	Melting Point (˚C)
95-57-8	2-Chlorophenol	9.8	72-55-9	DDE	89
84-74-2	Di-*n*-butyl phthalate	-35	50-29-3	DDT	108.5
95-50-1	1,2-Dichlorobenzene	-16.7	53-70-3	Dibenzo(*a,h*)anthracene	269.5
75-34-3	1,1-Dichloroethane	-96.9	106-46-7	1,4-Dichlorobenzene	52.7
107-06-2	1,2-Dichloroethane	-35.5	91-94-1	3,3-Dichlorobenzidine	132.5
75-35-4	1,1-Dichloroethylene	-122.5	120-83-2	2,4-Dichlorophenol	45
156-59-2	*cis*-1,2-Dichloroethylene	-80	60-57-1	Dieldrin	175.5
156-60-5	*trans*-1,2-Dichloroethylene	-49.8	105-67-9	2,4-Dimethylphenol	24.5
78-87-5	1,2-Dichloropropane	-70	51-28-5	2,4-Dinitrophenol	115-116
542-75-6	1,3-Dichloropropene	NA	121-14-2	2,4-Dinitrotoluene	71
84-66-2	Diethylphthalate	-40.5	606-20-2	2,6-Dinitrotoluene	66
117-84-0	Di-*n*-octyl phthalate	-30	72-20-8	Endrin	200
100-41-4	Ethylbenzene	-94.9	206-44-0	Fluoranthene	107.8
87-68-3	Hexachloro-1,3-butadiene	-21	86-73-7	Fluorene	114.8
77-47-4	Hexachlorocyclopentadiene	-9	76-44-8	Heptachlor	95.5
78-59-1	Isophorone	-8.1	1024-57-3	Heptachlor epoxide	160
74-83-9	Methyl bromide	-93.7	118-74-1	Hexachlorobenzene	231.8
75-09-2	Methylene chloride	-95.1	319-84-6	α-HCH (α-BHC)	160
98-95-3	Nitrobenzene	5.7	319-85-7	ß-HCH (ß-BHC)	315
100-42-5	Styrene	-31	58-89-9	γ-HCH (Lindane)	112.5
79-34-5	1,1,2,2-Tetrachloroethane	-43.8	67-72-1	Hexachloroethane	187
127-18-4	Tetrachloroethylene	-22.3	193-39-5	Indeno(1,2,3-*cd*)pyrene	161.5
108-88-3	Toluene	-94.9	72-43-5	Methoxychlor	87
120-82-1	1,2,4-Trichlorobenzene	17	95-48-7	2-Methylphenol	29.8
71-55-6	1,1,1-Trichloroethane	-30.4	621-64-7	*N*-Nitrosodi-*n*-propylamine	NA
79-00-5	1,1,2-Trichloroethane	-36.6	86-30-6	*N*-Nitrosodiphenylamine	66.5
79-01-6	Trichloroethylene	-84.7	91-20-3	Naphthalene	80.2
108-05-4	Vinyl acetate	-93.2	87-86-5	Pentachlorophenol	174
75-01-4	Vinyl chloride	-153.7	108-95-2	Phenol	40.9
108-38-3	*m*-Xylene	-47.8	129-00-0	Pyrene	151.2
95-47-6	*o*-Xylene	-25.2	8001-35-2	Toxaphene	65-90
106-42-3	*p*-Xylene	13.2	95-95-4	2,4,5-Trichlorophenol	69
			88-06-2	2,4,6-Trichlorophenol	69
			115-29-7	Endosullfan	106

NA = Not available.

When free phase liquid contaminants are suspected, *Estimating the Potential for Occurrence of DNAPL at Superfund Sites* (U.S. EPA, 1992c) provides information on determining the likelihood of dense nonaqueous phase liquid (DNAPL) occurrence in the subsurface. Free-phase contaminants may also be present at concentrations lower than C_{sat} if multiple component mixtures are present. The DNAPL guidance (U.S. EPA, 1992c) also addresses the likelihood of free-phase contaminants when multiple contaminants are present at a site.

For compounds that are solid at ambient soil temperatures (e.g., DDT), Table 3-A indicates that the inhalation risks are well below the screening targets (i.e., these chemicals do not appear to be of concern for the inhalation pathway). Thus, when inhalation SSLs are above C_{sat} for solid compounds, soil screening decisions should be based on the appropriate SSLs for other pathways of concern at the site (e.g., migration to ground water, ingestion).

2.4.5 Particulate Emission Factor. The particulate emission factor relates the concentration of contaminant in soil with the concentration of dust particles in the air. This guidance addresses dust generated from open sources, which is termed "fugitive" because it is not discharged into the atmosphere in a confined flow stream. Other sources of fugitive dusts that may lead to higher emissions due to mechanical disturbances include unpaved roads, tilled agricultural soils, and heavy construction operations.

Both the emissions portion and the dispersion portion of the PEF equation have been updated since RAGS HHEM, Part B.

As in Part B, the emissions part of the PEF equation is based on the "unlimited reservoir" model from Cowherd et al. (1985) developed to estimate particulate emissions due to wind erosion. The unlimited reservoir model is most sensitive to the threshold friction velocity, which is a function of the mode of the size distribution of surface soil aggregates. This parameter has the greatest effect on the emissions and resulting concentration. For this reason, a conservative mode soil aggregate size of 500 µm was selected as the default value for calculating generic SSLs.

The mode soil aggregate size determines how much wind is needed before dust is generated at a site. A mode soil aggregate size of 500 µm yields an **uncorrected** threshold friction velocity of 0.5 m/s. This means that the windspeed must be at least 0.5 m/s before any fugitive dusts are generated. However, the threshold friction velocity **should be corrected** to account for the presence of nonerodible elements. In Cowherd et al. (1985), nonerodible elements are described as

> . . . clumps of grass or stones (larger than about 1 cm in diameter) on the surface (that will) consume part of the shear stress of the wind which otherwise would be transferred to erodible soil.

Cowherd et al. describe a study by Marshall (1971) that used wind tunnel studies to quantify the increase in the threshold friction velocity for different kinds of nonerodible elements. His results are presented in Cowherd et al. as a graph showing the rate of corrected to uncorrected threshold friction velocity vs. L_c, where L_c is a measure of nonerodible elements vs. bare, loose soil. Thus, the ratio of corrected to uncorrected threshold friction velocity is directly related to the amount of nonerodible elements in surface soils.

Using a ratio of corrected to uncorrected threshold friction velocity of 1, or no correction, is roughly equivalent to modeling "coal dust on a concrete pad," whereas using a correction factor of 2 corresponds to a windspeed of 19 m/s at a height of 10 m. This means that about a 43-mph wind would be required to produce any particulate emissions. Given that the 29 meteorologic data sets used in this modeling effort showed few windspeeds at, or greater than, 19 m/s, EPA felt that it was necessary to choose a default correction ratio between 1 and 2. A value of 1.25 was selected as a reasonable number that would be at the more conservative end of the range. This equates to a corrected threshold friction velocity of 0.625 m/s and an equivalent windspeed of 11.3 m/s at a height of 7 meters.

As with the VF model, Q/C values are needed to calculate the PEF (Equation 10); use the QC value in Table 3 that best represents a site's size and meteorologic conditions (i.e., the same value used to calculate the VF; see Section 2.4.2). Cowherd et al. (1985) describe how to obtain site-specific estimates of V, U_m, U_t, and F(x).

Unlike volatile contaminants, meteorologic conditions (i.e., the intensity and frequency of wind) affect both the dispersion and emissions of particulate matter. For this reason, a separate default Q/C value was derived for particulate matter [nominally 10 µm and less (PM_{10})] emissions for the generic SSLs. The PEF equation was used to calculate annual average concentrations for each of 29 sites across the country. To develop a reasonably conservative default Q/C for calculating generic SSLs, a default site (Minneapolis, MN) was selected that best approximated the 90th percentile concentration.

The results produced a revised default PEF Q/C value of 90.80 g/m^2-s per kg/m^3 for a 0.5-acre site (see Appendix D; EQ, 1994). The generic PEF derived using the default values in Equation 10 is 1.32×10^9 m^3/kg, which corresponds to a receptor point concentration of approximately 0.76 $\mu g/m^3$. This represents an annual average emission rate based on wind erosion that should be compared with chronic health criteria; it is **not** appropriate for evaluating the potential for more acute exposures.

Derivation of the Particulate Emission Factor

$$\text{PEF }(m^3/kg) = Q/C \times \frac{3{,}600\ s/h}{0.036 \times (1-V) \times (U_m/U_t)^3 \times F(x)} \qquad \textbf{(10)}$$

Parameter/Definition (units)	Default	Source
PEF/particulate emission factor (m^3/kg)	1.32×10^9	--
Q/C/inverse of mean conc. at center of square source (g/m^2-s per kg/m^3)	90.80	Table 3 (for 0.5-acre source in Minneapolis, MN)
V/fraction of vegetative cover (unitless)	0.5 (50%)	U.S. EPA, 1991b
U_m/mean annual windspeed (m/s)	4.69	EQ, 1994
U_t/equivalent threshold value of windspeed at 7 m (m/s)	11.32	U.S. EPA, 1991b
F(x)/function dependent on U_m/U_t derived using Cowherd et al. (1985) (unitless)	0.194	U.S. EPA, 1991b

2.5 Migration to Ground Water

The methodology for calculating SSLs for the migration to ground water pathway was developed to identify chemical concentrations in soil that have the potential to contaminate ground water.

Migration of contaminants from soil to ground water can be envisioned as a two-stage process: (1) release of contaminant in soil leachate and (2) transport of the contaminant through the underlying soil and aquifer to a receptor well. The SSL methodology considers both of these fate and transport mechanisms.

The methodology incorporates a standard linear equilibrium soil/water partition equation to estimate contaminant release in soil leachate (see Sections 2.5.1 through 2.5.4) and a simple water-balance equation that calculates a dilution factor to account for dilution of soil leachate in an aquifer (see Section 2.5.5). The dilution factor represents the reduction in soil leachate contaminant concentrations by mixing in the aquifer, expressed as the ratio of leachate concentration to the concentration in ground water at the receptor point (i.e., drinking water well). Because the infinite source assumption can result in mass-balance violations for soluble contaminants and small sources, mass-limit models are provided that limit the amount of contaminant migrating from soil to ground water to the total amount of contaminant present in the source (see Section 2.6).

SSLs are backcalculated from acceptable ground water concentrations (i.e., nonzero MCLGs, MCLs, or HBLs; see Section 2.1). First, the acceptable ground water concentration is multiplied by a dilution factor to obtain a target leachate concentration. For example, if the dilution factor is 10 and the acceptable ground water concentration is 0.05 mg/L, the target soil leachate concentration would be 0.5 mg/L. The partition equation is then used to calculate the total soil concentration (i.e., SSL) corresponding to this soil leachate concentration.

The methodology for calculating SSLs for the migration to ground water pathway was developed under the following constraints:

- Because of the large nationwide variability in ground water vulnerability, the methodology should be flexible, allowing adjustments for site-specific conditions if adequate information is available.
- To be appropriate for early-stage application, the methodology needs to be simple, requiring a minimum of site-specific data.
- The methodology should be consistent with current understanding of subsurface processes.
- The process of developing and applying SSLs should generate information that can be used and built upon as a site evaluation progresses.

Flexibility is achieved by using readily obtainable site-specific data in standardized equations; conservative default input parameters are also provided for use when site-specific data are not available. In addition, more complex unsaturated zone fate-and-transport models have been identified that can be used to calculate SSLs when more detailed site-specific information is available or can be obtained (see Part 3). These models can extend the applicability of SSLs to subsurface conditions that are not adequately addressed by the simple equations (e.g., deep water tables; clay layers or other unsaturated zone characteristics that can attenuate contaminants before they reach ground water).

The SSL methodology was designed for use during the early stages of a site evaluation when information about subsurface conditions may be limited. Because of this constraint, the methodology is based on conservative, simplifying assumptions about the release and transport of contaminants in the subsurface (see Highlight 2).

Highlight 2: Simplifying Assumptions for the Migration to Ground Water Pathway

- The source is infinite (i.e., steady-state concentrations will be maintained in ground water over the exposure period of interest).
- Contaminants are uniformly distributed throughout the zone of contamination.
- Soil contamination extends from the surface to the water table (i.e., adsorption sites are filled in the unsaturated zone beneath the area of contamination).
- There is no chemical or biological degradation in the unsaturated zone.
- Equilibrium soil/water partitioning is instantaneous and linear in the contaminated soil.
- The receptor well is at the edge of the source (i.e., there is no dilution from recharge downgradient of the site) and is screened within the plume.
- The aquifer is unconsolidated and unconfined (surficial).
- Aquifer properties are homogeneous and isotropic.
- There is no attenuation (i.e., adsorption or degradation) of contaminants in the aquifer.
- NAPLs are not present at the site.

Although simplified, the SSL methodology described in this section is theoretically and operationally consistent with the more sophisticated investigation and modeling efforts that are conducted to develop soil cleanup goals and cleanup levels for protection of ground water at Superfund sites. SSLs developed using this methodology can be viewed as evolving risk-based levels that can be refined as more site information becomes available. The early use of the methodology at a site will help focus further subsurface investigations on areas of true concern with respect to ground water quality and will provide information on soil characteristics, aquifer characteristics, and chemical properties that can be built upon as a site evaluation progresses.

2.5.1 Development of Soil/Water Partition Equation. The methodology used to estimate contaminant release in soil leachate is based on the Freundlich equation, which was developed to model sorption from liquids to solids. The basic Freundlich equation applied to the soil/water system is:

$$K_d = C_s / C_w^n \tag{11}$$

where

K_d = Freundlich soil/water partition coefficient (L/kg)
C_s = concentration sorbed on soil (mg/kg)
C_w = solution concentration (mg/L)
n = Freundlich exponent (dimensionless).

Assuming that adsorption is linear with respect to concentration (n=1)* and rearranging to backcalculate a sorbed concentration (C_s):

$$C_s = (K_d)\, C_w \tag{12}$$

For SSL calculation, C_w is the target soil leachate concentration.

Adjusting Sorbed Soil Concentrations to Total Concentrations. To develop a screening level for comparison with contaminated soil samples, the sorbed concentration derived above (C_s) must be related to the total concentration measured in a soil sample (C_t). In a soil sample, contaminants can be associated with the solid soil materials, the soil water, and the soil air as follows (Feenstra et al., 1991):

$$M_t = M_s + M_w + M_a \tag{13}$$

where

M_t = total contaminant mass in sample (mg)
M_s = contaminant mass sorbed on soil materials (mg)
M_w = contaminant mass in soil water (mg)
M_a = contaminant mass in soil air (mg).

Furthermore,

$$M_t = C_t\, \rho_b\, V_{sp}\ , \tag{14}$$

$$M_s = C_s\, \rho_b\, V_{sp}\ , \tag{15}$$

$$M_w = C_w\, \theta_w\, V_{sp}\ , \tag{16}$$

and

$$M_a = C_a\, \theta_a\, V_{sp}\ , \tag{17}$$

where

ρ_b = dry soil bulk density (kg/L)
V_{sp} = sample volume (L)
θ_w = water-filled porosity (L_{water}/L_{soil})
C_a = concentration on soil pore air (mg/L_{soil})
θ_a = air-filled soil porosity (L_{air}/L_{soil}).

For contaminated soils (with concentrations below C_{sat}), C_a may be determined from C_w and the dimensionless Henry's law constant (H') using the following relationship:

$$C_a = C_w\, H' \tag{18}$$

---

* The linear assumption will tend to overestimate sorption and underestimate desorption for most organics at higher concentrations (i.e., above 10^{-5} M for organics) (Piwoni and Banerjee, 1989).

thus

$$M_a = C_w\, H'\, \theta_a\, V_{sp} \tag{19}$$

Substituting into Equation 13:

$$C_t = \frac{C_s \rho_b + C_w \theta_w + C_w H' \theta_a}{\rho_b} \tag{20}$$

or

$$C_s = C_t - C_w \left(\frac{\theta_w + \theta_a H'}{\rho_b} \right) \tag{21}$$

Substituting into Equation 12 and rearranging:

Soil-Water Partition Equation for Migration to Ground Water Pathway: Inorganic Contaminants

$$C_t = C_w \left(K_d + \frac{\theta_w + \theta_a H'}{\rho_b} \right) \tag{22}$$

Parameter/Definition (units)	Default	Source
C_t/screening level in soil (mg/kg)	–	–
C_w/target soil leachate concentration (mg/L)	(nonzero MCLG, MCL, or HBL) × 20 DAF	Table 1 (nonzero MCLG, MCL); Section 2.5.6 (DAF for 0.5-acre source)
K_d/soil-water partition coefficient (L/kg)	chemical-specific	see Part 5
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.3 (30%)	U.S. EPA/ORD
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.13	$n - \theta_w$
n/total soil porosity (L_{pore}/L_{soil})	0.43	$1 - \rho_b / \rho_s$
ρ_b/dry soil bulk density (kg/L)	1.5	U.S. EPA, 1991b
ρ_s/soil particle density (kg/L)	2.65	U.S. EPA, 1991b
H'/dimensionless Henry's law constant	H × 41, where 41 is a conversion factor	U.S. EPA, 1991b
H/Henry's law constant (atm-m^3/mol)	chemical-specific	see Part 5

Equation 22 is used to calculate SSLs (total soil concentrations, C_t) corresponding to soil leachate concentrations (C_w) equal to the target contaminant soil leachate concentration. The equation assumes that soil water, solids, and gas are conserved during sampling. If soil gas is lost during sampling, θ_a should be assumed to be zero. Likewise, for inorganic contaminants except mercury, there is no significant vapor pressure and H' may be assumed to be zero.

The User's Guide (U.S. EPA, 1996) describes how to develop site-specific estimates of the soil parameters needed to calculate SSLs. Default soil parameter values for the partition equation are the same as those used for the VF equation (see Section 2.4.2) except for average water-filled soil porosity (θ_w). A conservative value (0.15) was used in the VF equation because the model is most sensitive to this parameter. Because migration to ground water SSLs are not particularly sensitive to soil water content (see Section 2.5.7), a value that is more typical of subsurface conditions (0.30) was used. This value is between the mean field capacity (0.20) of Class B soils (Carsel et al., 1988) and the saturated volumetric water content for loam (0.43).

K_d varies by chemical and soil type. Because of different influences on K_d values, derivations of K_d values for organic compounds and metals were treated separately in the SSL methodology.

2.5.2 Organic Compounds—Partition Theory. Past research has demonstrated that, for hydrophobic organic chemicals, soil organic matter is the dominant sorbing component in soil and that K_d is linear with respect to soil organic carbon content (OC) as long as OC is above a critical level (Dragun, 1988). Thus, K_d can be normalized with respect to soil organic carbon to K_{oc}, a chemical-specific partitioning coefficient that is independent of soil type, as follows:

$$K_d = K_{oc}\, f_{oc} \qquad \textbf{(23)}$$

where

K_{oc} = organic carbon partition coefficient (L/kg)
f_{oc} = fraction of organic carbon in soil (mg/mg)

Substituting into Equation 22:

Soil-Water Partition Equation for Migration to Ground Water Pathway: Organic Contaminants

$$C_t = C_w \left((K_{oc}\, f_{oc}) + \frac{\theta_w + \theta_a H'}{\rho_b} \right) \qquad \textbf{(24)}$$

Parameter/Definition (units)	Default	Source
C_t/screening level in soil mg/kg)	–	–
C_w/target leachate concentration (mg/L)	(nonzero MCLG, MCL, or HBL) × 20 DAF	Table 1 (MCL, nonzero MCLG); Section 2.5.6 (DAF for a 0.5-acre source)
K_{oc}/soil organic carbon-water partition coefficient (L/kg)	chemical-specific	see Part 5
f_{oc}/organic carbon content of soil (kg/kg)	0.002 (0.2%)	Carsel et al., 1988
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.3 (30%)	U.S. EPA/ORD
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.13	$n - \theta_w$
n/total soil porosity (L_{pore}/L_{soil})	0.43	$1 - \rho_b/\rho_s$
ρ_b/dry soil bulk density (kg/L)	1.5	U.S. EPA, 1991b
ρ_s/soil particle density (kg/L)	2.65	U.S. EPA, 1991b
H'/dimensionless Henry's law constant	H × 41, where 41 is a conversion factor	U.S. EPA, 1991b
H/Henry's law constant (atm-m^3/mol)	chemical-specific	see Part 5

Part 5 of this document provides K_{oc} values for organic chemicals and describes their development.

The critical organic carbon content, f_{oc}^* , represents OC below which sorption to mineral surfaces begins to be significant. This level is likely to be variable and to depend on both the properties of the soil and of the chemical sorbate (Curtis et al., 1986). Attempts to quantitatively relate f_{oc}^* to such properties have been made (see McCarty et al., 1981), but at this time there is no reliable method for estimating f_{oc}^* for specific chemicals and soils. Nevertheless, research has demonstrated that, for volatile halogenated hydrocarbons, f_{oc}^* is about 0.001, or 0.1 percent OC, for many low-carbon soils and aquifer materials (Piwoni and Banerjee, 1989; Schwarzenbach and Westall, 1981).

If soil OC is below this critical level, Equation 24 should be used with caution. This is especially true if soils contain significant quantities of fine-grained minerals with high sorptive properties (e.g., clays). If sorption to minerals is significant, Equation 24 will underpredict sorption and overpredict contaminant concentrations in soil pore water. However, this f_{oc}^* level is by no means the case for all soils; Abdul et al. (1987) found that, for certain organic compounds and aquifer materials, sorption was linear and could be adequately modeled down to $f_{oc} = 0.0003$ by considering K_{oc} alone.

For soils with significant inorganic and organic sorption (i.e., soils with $f_{oc} < 0.001$), the following equation has been developed (McCarty et al., 1981; Karickhoff, 1984):

$$K_d = (K_{oc}\, f_{oc}) + (K_{io}\, f_{io}) \tag{25}$$

where

K_{io} = soil inorganic partition coefficient
f_{io} = fraction of inorganic material
$f_{io} + f_{oc}$ = 1.

Although this equation is considered conceptually valid, K_{io} values are not available for the subject chemicals. Attempts to estimate K_{io} values by relating sorption on low-carbon materials to properties such as clay-size fraction, clay mineralogy, surface area, or iron-oxide content have not revealed any consistent correlations, and semiquantitative methods are probably years away (Piwoni and Banerjee, 1989). However, Piwoni and Banerjee developed the following empirical correlation (by linear regression, $r^2 = 0.85$) that can be used to estimate K_d values for hydrophobic organic chemicals from K_{ow} for low-carbon soils:

$$\log K_d = 1.01 \log K_{ow} - 0.36 \qquad \textbf{(26)}$$

where

K_{ow} = octanol/water partition coefficient.

The authors indicate that this equation should provide a K_d estimate that is within a factor of 2 or 3 of the actual value for nonpolar sorbates with $\log K_{ow} < 3.7$. This K_d estimate can be used in Equation 22 for soils with f_{oc} values less than 0.001. If sorption to inorganics is not considered for low-carbon soils where it is significant, Equation 24 will underpredict sorption and overpredict contaminant concentrations in soil pore water (i.e., it will provide a conservative estimate).

The use of fixed K_{oc} values in Equation 24 is valid only for hydrophobic, nonionizing organic chemicals. Several of the organic chemicals of concern ionize in the soil environment, existing in both neutral and ionized forms within the normal soil pH range. The relative amounts of the ionized and neutral species are a function of pH. Because the sorptive properties of these two forms differ, it is important to consider the relative amounts of the neutral and ionized species when determining K_{oc} values at a particular pH. Lee et al. (1990) developed a theoretically based algorithm, developed from thermodynamic equilibrium equations, and demonstrated that the equation adequately predicts laboratory-measured K_{oc} values for pentachlorophenol (PCP) and other ionizing organic acids as a function of pH.

The equation assumes that sorbent organic carbon determines the extent of sorption for both the ionized and neutral species and predicts the overall sorption of a weak organic acid ($K_{oc,p}$) as follows:

$$K_{oc,p} = K_{oc,n}\,\Phi_n + K_{oc,i}\,(1 - \Phi_n) \qquad \textbf{(27)}$$

where

$K_{oc,n}$, $K_{oc,i}$ = sorption coefficients for the neutral and ionized species (L/kg)
Φ_n = $(1 + 10^{pH - pKa})^{-1}$
pKa = acid dissociation constant.

This equation was used to develop K_{oc} values for ionizing organic acids as a function of pH, as described in Part 5. The User's Guide (U.S. EPA, 1996) provides guidance on conducting site-specific measurements of soil pH for estimating K_{oc} values for ionizing organic compounds. Because a national distribution of soil pH values is not available, a median U.S. ground water pH (6.8) from the STORET database (U.S. EPA, 1992a) is used as a default soil pH value that is representative of subsurface pH conditions.

2.5.3 Inorganics (Metals)—Partition Theory.

Equation 22 is used to estimate SSLs for metals for the migration to ground water pathway. The derivation of K_d values is much more complicated for metals than for organic compounds. Unlike organic compounds, for which K_d values are largely controlled by a single parameter (soil organic carbon), K_d values for metals are significantly affected by a variety of soil conditions. The most significant parameters are pH, oxidation-reduction conditions, iron oxide content, soil organic matter content, cation exchange capacity, and major ion chemistry. The number of significant influencing parameters, their variability in the field, and differences in experimental methods result in a wide range of K_d values for individual metals reported in the literature (over 5 orders of magnitude). Thus, it is much more difficult to derive generic K_d values for metals than for organics.

The K_d values used to generate SSLs for Ag, Ba, Be, Cd, Cr^{+3}, Cu, Hg, Ni, and Zn were developed using an equilibrium geochemical speciation model (MINTEQ2). The values for As, Cr^{6+}, Se, and Th were taken from empirical, pH-dependent adsorption relationships developed by EPA/ORD. Metal K_d values for SSL application are presented in Part 5, along with a description of their development and limitations. As with the ionizing organics, K_d values are selected as a function of site-specific soil pH, and metal K_d values corresponding to a pH of 6.8 are used as defaults where site-specific pH measurements are not available.

2.5.4 Assumptions for Soil/Water Partition Theory.

The following assumptions are implicit in the SSL partitioning methodology. *These assumptions and their implications for SSL accuracy should be read and understood before using this methodology to calculate SSLs.*

1. **There is no contaminant loss due to volatilization or degradation.** The source is considered to be infinite; i.e., these processes do not reduce soil leachate concentrations over time. This is a **conservative** assumption, especially for smaller sites.

2. **Adsorption is linear with concentration.** The methodology assumes that adsorption is independent of concentration (i.e., the Freundlich exponent = 1). This has been reported to be true for various halogenated hydrocarbons, polynuclear aromatic hydrocarbons, benzene, and chlorinated benzenes. In addition, this assumption is valid at low concentrations (e.g., at levels close to the MCL) for most chemicals. As concentrations increase, however, the adsorption isotherm can depart from the linear.

   Studies on trichloroethane (TCE) and chlorobenzene indicate that departure from linear is in the **nonconservative** direction, with adsorbed concentrations being lower than predicted by a linear isotherm. However, adequate information is not available to establish nonlinear adsorption isotherms for the chemicals of interest. Furthermore, since the SSLs are derived at relatively low target soil leachate concentrations, departures from the linear at high concentrations do not significantly influence the accuracy of the results.

3. **The system is at equilibrium with respect to adsorption.** This ignores adsorption/desorption kinetics by assuming that the soil and pore water concentrations are at equilibrium levels. In other words, the pore-water residence time is assumed to be longer than the time it takes for the system to reach equilibrium conditions.

   This assumption is **conservative**. If equilibrium conditions are not met, the concentration in the pore water will be less than that predicted by the methodology. The kinetics of adsorption are not adequately understood for a sufficient number of chemicals and site conditions to consider equilibrium kinetics in the methodology.

4. **Adsorption is reversible.** The methodology assumes that desorption processes operate in the same way as adsorption processes, since most of the K_{oc} values are measured by adsorption experiments rather than by desorption experiments. In actuality, desorption is slower to some degree than adsorption and, in some cases, organics can be irreversibly bound to the soil matrix. In general, the significance of this effect increases with K_{ow}.

   This assumption is **conservative**. Slower desorption rates and irreversible sorption will result in lower pore-water concentrations than that predicted by the methodology. Again, the level of knowledge on desorption processes is not sufficient to consider desorption kinetics and degree of reversibility for all of the subject chemicals.

2.5.5 Dilution/Attenuation Factor Development. As contaminants in soil leachate move through soil and ground water, they are subjected to physical, chemical, and biological processes that tend to reduce the eventual contaminant concentration at the receptor point (i.e., drinking water well). These processes include adsorption onto soil and aquifer media, chemical transformation (e.g., hydrolysis, precipitation), biological degradation, and dilution due to mixing of the leachate with ambient ground water. The reduction in concentration can be expressed succinctly by a DAF, which is defined as the ratio of contaminant concentration in soil leachate to the concentration in ground water at the receptor point. When calculating SSLs, a DAF is used to backcalculate the target soil leachate concentration from an acceptable ground water concentration (e.g., MCLG). For example, if the acceptable ground water concentration is 0.05 mg/L and the DAF is 10, the target leachate concentration would be 0.5 mg/L.

The SSL methodology addresses only one of these dilution-attenuation processes: contaminant dilution in ground water. A simple equation derived from a geohydrologic water-balance relationship has been developed for the methodology, as described in the following subsection. The ratio factor calculated by this equation is referred to as a dilution factor rather than a DAF because it does not consider processes that attenuate contaminants in the subsurface (i.e., adsorption and degradation processes). This simplifying assumption was necessary for several reasons.

First, the infinite source assumption results in all subsurface adsorption sites being eventually filled and no longer available to attenuate contaminants. Second, soil contamination extends to the water table, eliminating attenuation processes in the unsaturated zone. Additionally, the receptor well is assumed to be at the edge of the source, minimizing the opportunity for attenuation in the aquifer. Finally, chemical-specific biological and chemical degradation rates are not known for many of the SSL chemicals; where they are available they are usually based on laboratory studies under simplified, controlled conditions. Because natural subsurface conditions such as pH, redox conditions, soil mineralogy, and available nutrients have been shown to markedly affect natural chemical and biological degradation rates, and because the national variability in these properties is significant and has not been characterized, EPA does not believe that it is possible at this time to incorporate these degradation processes into the simple site-specific methodology for national application.

If adsorption or degradation processes are expected to significantly attenuate contaminant concentrations at a site (e.g., for sites with deep water tables or soil conditions that will attenuate contaminants), the site manager is encouraged to consider the option of using more sophisticated fate and transport models. Many of these models can consider adsorption and degradation processes and can model transient conditions necessary to consider a finite source size. Part 3 of this document presents information on the selection and use of such models for SSL application.

The dilution factor model assumes that the aquifer is unconfined and unconsolidated and has homogeneous and isotropic properties. Unconfined (surficial) aquifers are common across the country, are vulnerable to contamination, and can be used as drinking water sources by local residents. Dilution model results may not be applicable to fractured rock or karst aquifer types. The site manager should consider use of more appropriate models to calculate a dilution factor (or DAF) for such settings.

In addition, the simple dilution model does not consider facilitated transport. This ignores processes such as colloidal transport, transport via solvents other than water (e.g., NAPLs), and transport via dissolved organic matter (DOM). These processes have greater impact as K_{ow} (and hence, K_{oc}) increases. However, the transport via solvents other than water is operative only if certain site-specific conditions are present. Transport by DOM and colloids has been shown to be potentially significant under certain conditions in laboratory and field studies. Although much research is in progress on these processes, the current state of knowledge is not adequate to allow for their consideration in SSL calculations.

If there is the potential for the presence of NAPLs in soils at the site or site area in question, SSLs should not be used for this area (i.e., further investigation is required). The C_{sat} equation (Equation 9) presented in Section 2.4.4 can be used to estimate the contaminant concentration at which the presence of pure-phase NAPLs may be suspected for contaminants that are liquid at soil temperature. If NAPLs are suspected in site soils, refer to U.S. EPA (1992c) for additional guidance on how to estimate the potential for DNAPL occurrence in the subsurface.

Dilution Model Development. EPA evaluated four simple water balance models to adjust SSLs for dilution in the aquifer. Although written in different terms, all four options reviewed can be expressed as the same simple water balance equation to calculate a dilution factor, as follows:

Option 1 (ASTM):

$$\text{dilution factor} = (1 + U_{gw}\, d/IL) \tag{28}$$

where

U_{gw} = Darcy ground water velocity (m/yr)
d = mixing zone depth (m)
I = infiltration rate (m/yr)
L = length of source parallel to flow (m).

For Darcy velocity:

$$U_{gw} = Ki \tag{29}$$

where

K = aquifer hydraulic conductivity (m/yr)
i = hydraulic gradient (m/m).

Thus

$$\text{dilution factor} = 1 + (Kid/IL) \tag{30}$$

Option 2 (EPA Ground Water Forum):

$$\text{dilution factor} = (Q_p + Q_A)/Q_p \qquad \textbf{(31)}$$

where

Q_p = percolation flow rate (m^3/yr)
Q_A = aquifer flow rate (m^3/yr)

For percolation flow rate:

$$Q_p = IA \qquad \textbf{(32)}$$

where

A = facility area (m^2) = WL.

For aquifer flow rate:

$$Q_A = WdKi \qquad \textbf{(33)}$$

where

W = width of source perpendicular to flow (m)
d = mixing zone depth (m).

Thus

$$\text{dilution factor} = (IA + WdKi)/IWL$$

$$= 1 + (Kid/IL) \qquad \textbf{(34)}$$

Option 3 (Summers Model):

$$C_w = (Q_p\, C_p)/(Q_p + Q_A) \qquad \textbf{(35)}$$

where

C_w = ground water contaminant concentration (mg/L)
C_p = soil leachate concentration (mg/L)

given that

$$C_w = C_p/\text{dilution factor}$$

$$1/\text{dilution factor} = Q_p/(Q_p + Q_A)$$

or

$$\text{dilution factor} = (Q_p + Q_A)/Q_p \text{ (see } \textbf{Option 2}\text{)}$$

Option 4 (EPA ORD/RSKERL):

$$\text{dilution factor} = (Q_p + Q_A)/Q_p = RX/RL \qquad \textbf{(36)}$$

where

R = recharge rate (m/yr) = infiltration rate (I, m/yr)
X = distance from receptor well to ground water divide (m)

(Note that the intermediate equation is the same as **Option 2**.)

This option is a longer-term option that is not considered further in this analysis because valid X values are not currently available either nationally or for specific sites. EPA is considering developing regional estimates for these parameters.

Dilution Model Input Parameters. As shown, all three options for calculating contaminant dilution in ground water can be expressed as the same equation:

Ground Water Dilution Factor

$$\text{dilution factor} = 1 + (Kid/IL) \qquad \textbf{(37)}$$

Parameter/Definition (units)
K/aquifer hydraulic conductivity (m/yr) i/hydraulic gradient (m/m) d/mixing zone depth (m) I/infiltration rate (m/yr) L/source length parallel to ground water flow (m)

Mixing Zone Depth (**d**). Because of its dependence on the other variables, mixing zone depth is estimated with the method used for the MULTIMED model (Sharp-Hansen et al., 1990). The MULTIMED estimation method was selected to be consistent with that used by EPA's Office of Solid Waste for the EPA Composite Model for Landfills (EPACML). The equation for estimating mixing zone depth (d) is as follows:

$$d = (2\alpha_v L)^{0.5} + d_a \{1 - \exp[(-LI)/(V_s n_e d_a)]\} \qquad \textbf{(38)}$$

where

α_v = vertical dispersivity (m/m)
V_s = horizontal seepage velocity (m/yr)
n_e = effective aquifer porosity ($L_{pore}/L_{aquifer}$)
d_a = aquifer depth (m).

The first term, $(2\alpha_v L)^{0.5}$, estimates the depth of mixing due to vertical dispersivity ($d_{\alpha v}$) along the length of ground water travel. Defining the point of compliance with ground water standards at the downgradient edge of the source, this travel distance becomes the length of the source parallel to flow L. Vertical dispersivity can be estimated by the following relationship (Gelhar and Axness, 1981):

$$\alpha_v = 0.056\ \alpha_L \tag{39}$$

where

α_L = longitudinal dispersivity = 0.1 x_r
x_r = horizontal distance to receptor (m).

Because the potential receptor is assumed to have a well at the edge of the facility, x_r = L and

$$\alpha_v = 0.0056\ L \tag{40}$$

Thus

$$d_{\alpha v} = (0.0112\ L^2)^{0.5} \tag{41}$$

The second term, $d_a\ \{1 - \exp[(-LI) / (V_s n_e d_a)]\}$, estimates the depth of mixing due to the downward velocity of infiltrating water, d_{Iv}. In this equation, the following substitution may be made:

$$V_s = Ki/n_e \tag{42}$$

so

$$d_{Iv} = d_a\ \{1 - \exp[(-LI)/(Kid_a)]\} \tag{43}$$

Thus, mixing zone depth is calculated as follows:

$$d = d_{\alpha v} + d_{Iv} \tag{44}$$

Estimation of Mixing Zone Depth

$$d = (0.0112\ L^2)^{0.5} + d_a\ \{1 - \exp[(-LI)/(Kid_a)]\} \tag{45}$$

Parameter/Definition (units)
d/mixing zone depth (m) L/source length parallel to ground water flow (m) I/infiltration rate (m/yr) K/aquifer hydraulic conductivity (m/yr) d_a/aquifer thickness (m)

Incorporation of this equation for mixing zone depth into the SSL dilution equation results in five parameters that must be estimated to calculate dilution: source length (L), infiltration rate (I), aquifer hydraulic conductivity (K), aquifer hydraulic gradient (i), and aquifer thickness (d_a). Aquifer thickness also serves as a limit for mixing zone depth. The User's Guide (U.S. EPA, 1996) describes how to develop site-specific estimates for these parameters. Parameter definitions and defaults used to develop generic SSLs are as follows:

- **Source Length (L)** is the length of the source (i.e., area of contaminated soil) parallel to ground water flow and affects the flux of contaminant released in soil leachate (IL) as well as the depth of mixing in the aquifer. The default option for this parameter assumes a square, 0.5-acre contaminant source. This default was changed from 30 acres in response to comments to be more representative of actual contaminated soil sources (see Section 1.3.4). Increasing source area (and thereby area) may result in a lower dilution factor. Appendix A includes an analysis of the conservatism associated with the 0.5-acre source size.

- **Infiltration Rate (I)**. Infiltration rate times the source area determines the amount of contaminant (in soil leachate) that enters the aquifer over time. Thus, increasing infiltration decreases the dilution factor. Two options can be used to generate infiltration rate estimates for SSL calculation. The first assumes that infiltration rate is equivalent to recharge. This is generally true for uncontrolled contaminated soil sites but would be conservative for capped sites (infiltration < recharge) and nonconservative for sites with an additional source of infiltration, such as surface impoundments (infiltration > recharge). Recharge estimates for this option can be obtained from Aller et al. (1987) by hydrogeologic setting, as described in Section 2.5.6.

  The second option is to use the HELP model to estimate infiltration, as was done for OSW's EPACML and EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP) modeling efforts. The Soil Screening Guidance (U.S. EPA, 1995c) provides information on obtaining and using the HELP model to estimate site-specific infiltration rates.

- **Aquifer Parameters**. Aquifer parameters needed for the dilution factor model include hydraulic conductivity (K, m/yr), hydraulic gradient (i, m/m), and aquifer thickness (d_a, m). The User's Guide (U.S. EPA, 1996) describes how to develop aquifer parameter estimates for calculating a site-specific dilution factor.

2.5.6 Default Dilution-Attenuation Factor. EPA has selected a default DAF of 20 to account for contaminant dilution and attenuation during transport through the saturated zone to a compliance point (i.e., receptor well). At most sites, this adjustment will more accurately reflect a contaminant's threat to ground water resources than assuming a DAF of 1 (i.e., no dilution or attenuation). EPA selected a DAF of 20 using a "weight of evidence" approach. This approach considers results from OSW's EPACMTP model as well as results from applying the SSL dilution model described in Section 2.5.5 to 300 ground water sites across the country.

The default DAF of 20 represents an adjustment from the DAF of 10 presented in the December 1994 draft Soil Screening Guidance (U.S. EPA, 1994h) to reflect a change in default source size from 30 acres to 0.05 acre. A DAF of 20 is protective for sources up to 0.5 acre in size. Analyses presented in Appendix A indicate that it can be protective of larger sources as well. However, this hypothesis should be examined on a case-by-case basis before applying a DAF of 20 to sources larger than 0.5 acre.

EPACMTP Modeling Effort. One model considered during selection of the default DAF is described in *Background Document for EPA's Composite Model for Leachate Migration with Transformation Products* (U.S. EPA, 1993a). EPACMTP has a three-dimensional module to simulate ground water flow that can account for mounding under waste sites. The model also has a three-dimensional transport module and both linear and nonlinear adsorption in the unsaturated and saturated zones and can simulate chain decay, thus allowing the simulation of the formation and the fate and transport of daughter (transformation) products of degrading chemicals. The model can also be used to simulate a finite source scenario.

EPACMTP is comprised of three main interconnected modules:

- An unsaturated zone flow and contaminant fate and transport module
- A saturated zone ground water flow and contaminant fate and transport module
- A Monte Carlo driver module, which generates model parameters from nationwide probability distributions.

The unsaturated and saturated zone modules simulate the migration of contaminants from initial release from the soil to a downgradient receptor well. More information on the EPACMTP model is provided in Appendix E.

EPA has extensively verified both the unsaturated and saturated zone modules of the EPACMTP against other available analytical and numerical models to ensure accuracy and efficiency. Both the unsaturated zone and the saturated zone modules of the EPACMTP have been reviewed by the EPA Science Advisory Board and found to be suitable for generic applications such as the derivation of nationwide DAFs.

EPACMTP Model Inputs (SSL Application). For nationwide Monte Carlo model applications, the input to the model is in the form of probability distributions of each of the model input parameters. The output from the model consists of the probability distribution of DAF values, representing the likelihood that the DAF will not be less than a certain value. For instance, a 90th percentile DAF of 10 means that the DAF will be 10 or higher in at least 90 percent of the cases.

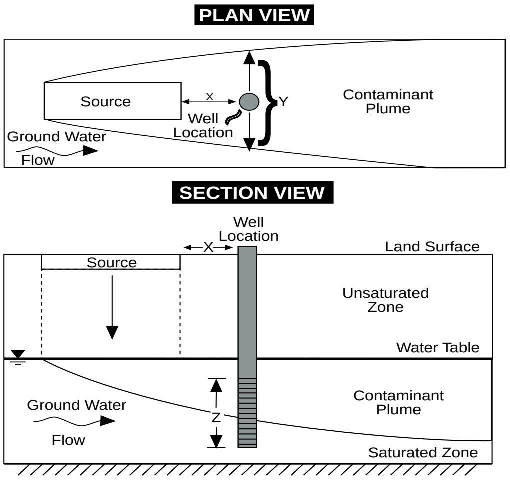
For each model input parameter, a probability distribution is provided, describing the nationwide likelihood that the parameter has a certain value. The parameters are divided into four main groups:

- Source-specific parameters, e.g., area of the waste unit, infiltration rate
- Chemical-specific parameters, e.g., hydrolysis constants, organic carbon partition coefficient

- Unsaturated zone-specific parameters, e.g., depth to water table, soil hydraulic conductivity

- Saturated zone-specific parameters, e.g., saturated zone thickness, ambient ground water flow rate, location of nearest receptor well.

Probability distributions for each parameter used in the model have been derived from nationwide surveys of waste sites, such as EPA's landfill survey (53 FR 28692). During the Monte Carlo simulation, values for each model parameter are randomly drawn from their respective probability distributions. In the calculation of the DAFs for generic SSLs, site data from over 1,300 municipal landfill sites in OSW's Subtitle D Landfill Survey were used to define parameter ranges and distributions. Each combination of randomly drawn parameter values represents one out of a practically infinite universe of possible waste sites. The fate and transport modules are executed for the specific set of model parameters, yielding a corresponding DAF value. This procedure is repeated, typically on the order of several thousand times, to ensure that the entire universe of possible parameter combinations (waste sites) is adequately sampled. In the derivation of DAFs for generic SSLs, the model simulations were repeated 15,000 times for each scenario investigated. At the conclusion of the analysis, a cumulative frequency distribution of DAF values was constructed and plotted.



Parameters:

- X (distance from source to well) = 0 ft
- Y (transverse well location) = Monte Carlo within 1/2 width of source
- Z (well intake point below water table) = Monte Carlo, range 15 → 300 ft
- Rainfall = Monte Carlo
- Soil type = Monte Carlo
- Depth to aquifer = Monte Carlo
- Assumes infinite source term

Figure 3. Migration to ground water pathway—EPACMTP modeling effort.

EPA assumed an infinite waste source of fixed area for the generic SSL modeling scenario. EPA chose this relatively conservative assumption because of limited information on the nationwide distribution of the volumes of contaminated soil sources. For the SSL modeling scenario, EPA performed a number of sensitivity analyses consisting of fixing one parameter at a time to determine the parameters that have the greatest impact on DAFs. The results of the sensitivity analyses indicate that the climate (net precipitation), soil types, and size of the contaminated area have the greatest effect on the DAFs. The EPA feels that the size of the contaminated area lends itself most readily to practical application to SSLs.

To calculate DAFs for the SSL scenario, the receptor point was taken to be a domestic drinking water well located on the downgradient edge of the contaminated area. The location of the intake point (receptor well screen) was assumed to vary between 15 and 300 feet below the water table (these values are based on empirical data reflecting a national sample distribution of depth of residential drinking water wells). The location of the intake point allows for mixing within the aquifer. EPA believes that this is a reasonable assumption because there will always be some dilution attributed to the pumping of water for residential use from an aquifer. The horizontal placement of the well was assumed to vary uniformly along the center of the downgradient edge of the source within a width of one-half of the width of the source. Degradation and retardation of contaminants were not considered in this analysis. Figure 3 is a schematic showing aspects of the subsurface SSL conceptual model used in the EPACMTP modeling effort. Appendix E is the background document prepared by EPA/OSW for this modeling effort.

EPACMTP Model Results. The results of the EPACMTP analyses indicate a DAF of about 170 for a 0.5-acre source at the 90th percentile protection level (Table 5). If a 95th percentile protection level is used, a DAF of 7 is protective for a 0.5-acre source.

Table 5. Variation of DAF with Size of Source Area for SSL EPACMTP Modeling Effort

	DAF		
Area (acres)	**85th**	**90th**	**95th**
0.02	1.42E+07	2.09E+05	946
0.04	9.19E+05	2.83E+04	211
0.11	5.54E+04	2.74E+03	44
0.23	1.16E+04	644	15
0.50	2.50E+03	170	7.0
0.69	1.43E+03	120	4.5
1.1	668	60	3.1
1.6	417	38	2.5
1.8	350	33	2.3
3.4	159	18	1.7
4.6	115	13	1.6
11.5	41	5.5	1.2
23	21	3.5	1.2
30	16	3.0	1.1
46	12	2.4	1.1
69	8.7	2.0	1.1

Dilution Factor Modeling Effort. To gain further information on the national range and distribution of DAF values, EPA also applied the simple SSL water balance dilution model to ground water sites included in two large surveys of hydrogeologic site investigations. These were American Petroleum Institute's (API's) hydrogeologic database (HGDB) and EPA's database of conditions at Superfund sites contaminated with DNAPL.

The HGDB contains the results of a survey sponsored by API and the National Water Well Association (NWWA) to determine the national variability in simple hydrogeologic parameters (Newell et al., 1989). The survey was conducted to validate EPA's use of the EPACML model as a screening tool for the land disposal of hazardous wastes. The survey involved more than 400 ground water professionals who submitted data on aquifer characteristics from field investigations at actual waste sites and other ground water projects. The information was compiled in HGDB, which is available from API and is included in OASIS, an EPA-sponsored ground water decision support system. Newell et al. (1990) also present these data as "national average" conditions and by hydrogeologic settings based on those defined by Aller et al. (1987) for the DRASTIC modeling effort. Aller et al. (1987) defined these settings within the overall framework defined by Heath's ground water regions (Heath, 1984). The HGDB estimates of hydraulic conductivity and hydraulic gradient show reasonable agreement with those in Aller et al. (1987), which serves as another source of estimates for these parameters.

The SSL dilution factor model (including the associated mixing zone depth model) requires estimates for five parameters:

d_a = aquifer thickness (m)
L = length of source parallel to flow (m)
I = infiltration rate (m/yr)
K = aquifer hydraulic conductivity (m/yr)
i = hydraulic gradient (m/m).

Dilution factors were calculated by individual HGDB or DNAPL site to retain as much site-correlated parameter information as possible. The HGDB contains estimates of aquifer thickness (d_a), aquifer hydraulic conductivity (K), and aquifer hydraulic gradient (i) for 272 ground water sites. The aquifer hydraulic conductivity estimates were examined for these sites, and sites with reported values less than 5×10^{-5} cm/s were culled from the database because formations with lower hydraulic conductivity values are not likely to be used as drinking water sources. In addition, sites in fractured rock or solution limestone settings were removed because the dilution factor model does not adequately address such aquifers. This resulted in 208 sites remaining in the HGDB. The DNAPL site database contains 92 site estimates of seepage velocity ($\bar{v}$), which can be related to hydraulic conductivity and hydraulic gradient by the following relationship:

$$\bar{v} = Ki / n_e \tag{46}$$

where

n_e = effective porosity.

Effective porosity (n_e) was assumed to be 0.35, which is representative of sand and gravel aquifers (the most prevalent aquifer type in the HGDB). Thus, for the DNAPL sites, $0.35 \times \bar{v}$ was substituted for Ki in the dilution factor equation.

Estimates of the other parameters required for the modeling effort are described below. Site-specific values were used where available. Because the modeling effort uses a number of site-specific modeling results to determine a nationwide distribution of dilution factors, typical values were used to estimate parameters for sites without site-specific estimates.

Source Length (L). The contaminant source (i.e., area of soil contamination) was assumed to be square. This assumption may be conservative for sites with their longer dimensions perpendicular to ground water flow or nonconservative for sites with their longer dimensions parallel to ground water flow. The source length was calculated as the square root of the source area for the source sizes in question. To cover a range of contaminated soil source area sizes, five source sizes were modeled: 0.5 acre, 10 acres, 30 acres, 60 acres, and 100 acres.

Infiltration Rate (I). Infiltration rate estimates were not available in either database. Recharge estimates for individual hydrogeologic settings from Aller et al. (1987) were used as infiltration estimates (i.e., it was assumed that infiltration = recharge). Because of differences in database contents, it was necessary to use different approaches to obtaining recharge/infiltration estimates for the HGDB and DNAPL sites.

The HGDB places each of its sites in one of the hydrogeologic settings defined by Aller et al. (1987). A recharge estimate for each HGDB site was simply extracted for the appropriate setting from Aller et al. The median of the recharge range presented was used (Table 6).

The DNAPL database does not contain sufficient hydrogeologic information to place each site into the Aller et al. settings. Instead, each of the 92 DNAPL sites was placed in one of Heath's ground water regions. The sites were found to lie within five hydrogeologic regions: nonglaciated central, glaciated central, piedmont/blue ridge, northeast and superior uplands, and Atlantic/Gulf coastal plain. Recharge was estimated for each region by averaging the median recharge value from all hydrogeologic settings except for those with steep slopes. The appropriate Heath region recharge estimate was then used for each DNAPL site in the dilution factor calculations.

Aquifer Parameters. All aquifer parameters needed for the SSL dilution model are included in the HGDB. Because hydraulic conductivity and gradient are included in the seepage velocity estimates in the DNAPL site database, only aquifer thickness was unknown for these sites. Aquifer thickness for all DNAPL sites was set at 9.1 m, which is the median value for the "national average" condition in the HGDB (Newell et al., 1990).

Dilution Modeling Results. Table 7 presents summary statistics for the 92 DNAPL sites, the 208 HGDB sites, and all 300 sites. One can see that the HGDB sites generally have lower dilution factors than the DNAPL sites, although the absolute range in values is greater in the HGDB. However, the available information for these sites is insufficient to fully explain the differences in these data sets. The wide range of dilution factors for these sites reflects the nationwide variability in hydrogeologic conditions affecting this parameter. The large difference between the average and geometric mean statistics indicates a distribution skewed toward the lower dilution factor values. The geometric mean represents a better estimate of the central tendency of such skewed distributions. Appendix F presents the dilution modeling inputs and results for the HGDB and DNAPL sites, tabulated by individual site.

Selection of the Default DAF. The default DAF was selected considering the evidence of the national DAF and dilution factor estimates described above. A DAF of 10 was selected in the December 1994 draft Soil Screening Guidance to be protective of a 30-acre source size. The EPACMTP model results showed a DAF of 3 for 30 acres at the 90th percentile. The SSL dilution model results have geometric mean dilution factors for a 30-acre source of 10 and 7 for DNAPL sites and HGDB sites, respectively. In a weight of evidence approach, more weight was given to the results of the DNAPL sites because they are representative of the kind of sites to which SSLs are likely to be applied. Considering the conservative assumptions in the SSL dilution factor model (see Section 2.5.5), and the conservatism inherent in the soil partition methodology (see Section 2.5.4), EPA believes (1) that these results support the use of a DAF of 10 for a 30-acre source, and (2) that this DAF will protect human health from exposure through this pathway at most Superfund sites across the Nation

Table 6. Recharge Estimates for DNAPL Site Hydrogeologic Regions

	Recharge (m/yr)		
Hydrogeologic setting	Min.	Max.	Avg.
Nonglaciated Central (Region 6)			
Alluvial Mountain Valleys	0.10	0.18	0.14
Alter. SS/LS/Sh., Thin Soil	0.10	0.18	0.14
Alter. SS/LS/Sh., Deep Regolith	0.10	0.18	0.14
Solution Limestone*	0.25	0.38	0.32
Alluvium w/ Overbank Deposits	0.18	0.25	0.22
Alluvium w/o Overbank Deposits	0.18	0.25	0.22
Braided River Deposits	0.10	0.18	0.14
Triassic Basins	0.10	0.18	0.14
Swamp/Marsh	0.10	0.18	0.14
Met./Ig. Domes & Fault Blocks	0.00	0.05	0.03
Unconsol./Semiconsol. Aquifers	0.00	0.05	0.03
	Overall Average:		*0.15*
Glaciated Central (Region 7)			
Glacial Till Over Bedded Rock	0.10	0.18	0.14
Glacial Till Over Outwash	0.10	0.18	0.14
Glacial Till Over Sol. Limestone	0.10	0.18	0.14
Glacial Till Over Sandstone	0.10	0.18	0.14
Glacial Till Over Shale	0.10	0.18	0.14
Outwash	0.18	0.25	0.22
Outwash Over Bedded Rock*	0.25	0.38	0.32
Outwash Over Solution Limestone*	0.25	0.38	0.32
Moraine	0.18	0.25	0.22
Buried Valley	0.18	0.25	0.22
Alluvium w/ Overbank Deposits	0.10	0.18	0.14
Alluvium w/o Overbank Deposits*	0.25	0.38	0.32
Glacial Lake Deposits	0.10	0.18	0.14
Thin Till Over Bedded Rock	0.18	0.25	0.22
Beaches, B. Ridges, Dunes*	0.25	0.38	0.32
Swamp/Marsh	0.10	0.18	0.14
	Overall Average:		*0.20*
Piedmont/Blue Ridge (Region 8)			
Alluvial Mountain Valleys	0.18	0.25	0.22
Regolith	0.10	0.18	0.14
River Alluvium	0.18	0.25	0.22
Mountain Crests	0.00	0.05	0.03
Swamp/Marsh	0.10	0.18	0.14
	Overall Average:		*0.15*
Northeast & Superior Uplands (Region 9)			
Alluvial Mountain Valleys	0.18	0.25	0.22
Till Over Crystalline Bedrock	0.18	0.25	0.22
Glacial Till Over Outwash	0.18	0.25	0.22
Outwash*	0.25	0.38	0.32
Moraine	0.18	0.25	0.22
Alluvium w/ Overbank Deposits	0.18	0.25	0.22
Alluvium w/o Overbank Deposits*	0.25	0.38	0.32
Swamp/Marsh	0.10	0.18	0.14
Bedrock Uplands	0.10	0.18	0.14
Glacial Lake/Marine Deposits	0.10	0.18	0.14
Beaches, B. Ridges, Dunes*	0.25	0.38	0.32
	Overall Average:		*0.22*
Atlantic/Gulf Coastal Plain (Region 10)			
Regional Aquifers	0.00	0.05	0.03
Un./Semiconsol. Surficial Aquifer*	0.25	0.38	0.32
Alluvium w/ Overbank Deposits	0.18	0.25	0.22
Alluvium w/o Overbank Deposits*	0.25	0.38	0.32
Swamp*	0.25	0.38	0.32
	Overall Average:		*0.24*

Source: Aller et al. (1987); hydrogeologic regions from Heath (1984).

** 0.25 m to 0.38 m (9.8 in to 15 in) used as recharge range for 25+ m setting values from Aller et al. (1987).*

Table 7. SSL Dilution Factor Model Results: DNAPL and HGDB Sites

	Source area (acres)				
	0.5	**10**	**30**	**100**	**600**
DNAPL Sites (92)					
Geomean	34	15	10	6	4
Average	321	138	80	44	19
10th percentile	3	2	1	1	1
25th percentile	8	4	3	2	1
Median	30	13	8	5	3
75th percentile	140	60	35	20	9
90th percentile	336	144	84	46	20
HGDB sites (208)					
Geomean	16	10	7	5	3
Average	958	829	561	371	159
10th percentile	2	1	1	1	1
25th percentile	3	2	1	1	1
Median	10	6	5	3	2
75th percentile	56	30	19	12	5
90th percentile	240	134	90	51	21
All 300 sites					
Geomean	20	11	8	6	3
Average	763	617	414	271	116
10th percentile	2	1	1	1	1
25th percentile	4	2	2	1	1
Median	15	8	5	4	2
75th percentile	70	35	23	13	6
90th percentile	292	144	88	49	21

DNAPL = DNAPL Site Survey (EPA/OERR).
HGDB = Hydrogeologic database (API).

To adjust the 30-acre DAF for a 0.5-acre source, EPA considered the geomean 0.5-acre dilution factors for the DNAPL sites (34), HGDB sites (16), and all 300 sites (20). A default DAF of 20 was selected as a conservative value for a 0.5-acre source size.

This value also reflects the ratio between 0.5-acre and 30-acre geomean and median dilution factors calculated for the HGDB sites (2.2 and 2.0, respectively). The HGDB data reflect the influence of source size on actual dilution factors more accurately than the DNAPL site data because the HGDB includes site-specific estimates of aquifer thickness. As shown in the following section, aquifer thickness has a strong influence on the effect of source size on the dilution factor since it provides an upper limit on mixing zone depth. Increasing source area increases infiltration, which lowers the dilution factor, but also increases mixing zone depth, which increases the dilution factor. For an infinitely thick aquifer, these effects tend to cancel each other, resulting in similar dilution factors for 0.5 and 30 acres. Thin aquifers limit mixing depth for larger sources; thus the added infiltration predominates and lowers the dilution factors for the larger source. Since the DNAPL dilution factor analyses use a fixed aquifer depth, they tend to overestimate the reduction in dilution factors that result from a smaller source.

2.5.7 Sensitivity Analysis. A sensitivity analysis was conducted to examine the effects of site-specific parameters on migration to ground water SSLs. Both the partition equation and the dilution factor model were considered in this analysis. Because an adequate database of national distributions of these parameters was not available, a nominal range method was used to conduct the analysis. In this analysis, independent parameters were selected and each was taken to maximum and minimum values while keeping all other parameters at their nominal, or default, values.

Overall, SSLs are most sensitive to changes in the dilution factor. As shown in Table 7, the 10th to 90th percentile dilution factors vary from 2 to 292 for the 300 DNAPL and HGDB sites. Much of this variability can be attributed to the wide range of aquifer hydraulic conductivity across the Nation. In contrast, the most sensitive parameter in the partition equation (f_{oc}) only affects the SSL by a factor of 1.5.

Partition Equation. The partition equation requires the following site-specific inputs: fraction organic carbon, average annual soil moisture content, and soil bulk density. Although volumetric soil moisture content is somewhat dependent on bulk density (in terms of the porosity available to be filled with water), calculations were conducted to ensure that the parameter ranges selected do not result in impossible combinations of these parameters. Because the effects of the soil parameters on the SSLs are highly dependent on chemical properties, the analysis was conducted on four organic chemicals spanning the range of these properties: chloroform, trichloroethylene, naphthalene, and benzo(*a*)pyrene.

The range used for soil moisture conditions was 0.02 to 0.43 L water/L soil. The lower end of this range represents a likely residual moisture content value for sand, as might be found in the drier regions of the United States. The higher value (0.43) represents full saturation conditions for a loam soil. The range of bulk density (1.25 to 1.75) was obtained from the Patriot soils database, which contains bulk density measurements for over 20,000 soil series across the United States.

Establishing a range for subsurface organic carbon content (f_{oc}) was more difficult. In spite of an extensive literature review and contacts with soil scientists, very little information was found on the distribution of this parameter with depth in U.S. soils. The range used was 0.001 to 0.003 g carbon / g soil. The lower limit represents the critical organic carbon content below which the partition equation is no longer applicable. The upper limit was obtained from EPA's Environmental Research Laboratory in Ada, Oklahoma, as an expert opinion. Generally, soil organic carbon content falls off rapidly with depth. Since the typical value used as an SSL default for surface soils is 0.006, and 0.002 is used for subsurface soils, this limited range is consistent with the other default assumptions used in the Soil Screening Guidance.

The results of the partition equation sensitivity analysis are shown in Table 8.

For volatile chemicals, the model is somewhat sensitive to water content, with up to 54 and 19 percent change in SSLs for chloroform and trichloroethylene, respectively. The model is less sensitive to bulk density, with a high percent change of 18 for chloroform and 14 for trichloroethylene. Organic carbon content has the greatest effect on SSLs for all chemicals except chloroform. As expected, the effect of f_{oc} increases with increasing K_{oc}. The greatest effect was seen for benzo(*a*)pyrene whose SSL showed a 50 percent increase at an f_{oc} of 0.03. An f_{oc} of 0.005 will increase the benzo(*a*)pyrene SSL by 150 percent.

Table 8. Sensitivity Analysis for SSL Partition Equation

Parameter assignments	Chloroform		Trichloroethylene		Naphthalene		Benzo(*a*)pyrene	
	SSL (mg/kg)	Percent change	SSL (mg/kg)	Percent change	SSL (mg/kg)	Percent change	SSL (mg/kg)	Percent change
All default parameter values	0.59	—	0.057	—	84	—	8	—
Less conservative parameter value								
Organic carbon	0.67	14	0.074	29	124	48	12	50
Bulk density	0.69	18	0.065	14	85	1	8	0
Soil moisture	0.74	26	0.062	9	86	2	8	0
More conservative parameter value								
Organic carbon	0.51	-14	0.040	-29	44	-48	4	-50
Bulk density	0.51	-13	0.051	-10	83	-1	8	0
Soil moisture	0.27	-54	0.046	-19	80	-4	8	0

Input parameters	Conservatism		
	Less	Nominal	More
Fraction org. carbon (g/g)	0.003	0.002	0.001
Bulk density (kg/L)	1.25[a]	1.50	1.75[b]
Average soil moisture (L/L)	0.43	0.30	0.02

[a] n = 0.53; q_a = 0.23.

[b] n = 0.34; q_a = 0.04.

Chemical-specific parameters	Chloroform	Trichloroethylene	Naphthalene	Benzo(*a*)pyrene
K_{oc}	3.98E+01	1.66E+02	2.00E+03	1.02E+06
H'	1.50E-01	4.22E-01	1.98E-02	4.63E-05
C_w	2.0[c]	0.1[c]	20[d]	0.004[c]

[c] MCL × 20 DAF.

[d] HBL (HQ=1) × 20 DAF.

Dilution Factor. Site-specific parameters for the dilution factor model include aquifer hydraulic conductivity (K), hydraulic gradient (i), infiltration rate (I), aquifer thickness (d), and source length parallel to ground water flow (L). Because they are somewhat dependent, hydraulic conductivity and hydraulic gradient were treated together as Darcy velocity (K × i). The parameter ranges used for the dilution factor analysis represent the 10th and 90th percentile values taken from the HGDB and DNAPL site databases, with the geometric mean serving as the nominal value, as shown in Table 9.

Source length was varied by assuming square sources of 0.5 to 30 acres in size. Bounding estimates were conducted for each of these source sizes.
The results in Table 9 show that Darcy velocity has the greatest effect on the dilution factor, with a range of dilution factors from 1.2 to 85 for a 30-acre source and 2.1 to 263 for a 0.5-acre source. Infiltration rate has the next highest effect, followed by source size and aquifer thickness. Note that aquifer thickness has a profound effect on the influence of source size on the dilution factor. Thick aquifers show no source size effect because the increase in infiltration flux from a larger source is balanced by the increase in mixing zone depth, which increases dilution in the aquifer. For very thin aquifers, the mixing zone depth is limited by the aquifer thickness and the increased infiltration flux predominates, decreasing the dilution factor for larger sources.

2.6 Mass-Limit Model Development

This section describes the development of models to solve the mass-balance violations inherent in the infinite source models used to calculate SSLs for the inhalation and migration to ground water exposure pathways. The models developed are not finite source models per se, but are designed for use with the current infinite source models to provide a lower, mass-based limit for SSLs for the migration to ground water and inhalation exposure pathways for volatile and leachable contaminants. For each pathway, the mass-limit model calculates a soil concentration that corresponds to the release of all contaminants present within the source, at a constant health-based concentration, over the duration of exposure. These mass-based concentration limits are used as a minimum concentration for each SSL; below this concentration, a receptor point concentration time-averaged over the exposure period cannot exceed the health-based concentration on which it is based.

2.6.1 Mass Balance Issues. Infinite source models are subject to mass balance violations under certain conditions. Depending on a compound's volatility and solubility and the size of the source, modeled volatilization or leaching rates can result in a source being depleted in a shorter time than the exposure duration (or the flux over a 30- or 70-year duration would release a greater mass of contaminants than are present). Several commenters to the December 1994 draft Soil Screening Guidance expressed concern that it is unrealistic for total emissions over the duration of exposure to exceed the total mass of contaminants in a source. Using the soil saturation concentration (C_{sat}) and a 5- to 10-meter contaminant depth, one commentor calculated that mass balance would be violated by the SSL volatilization model for 25 percent of the SSL chemicals.

Short of finite source modeling, the limitations of which in soil screening are discussed in the draft *Technical Background Document for Soil Screening Guidance* (U.S. EPA, 1994i), there were two options identified for addressing mass-balance violations within the soil screening process:

- Shorten the exposure duration to a value that would reflect mass limitations given the volatilization rate calculated using the current method

Table 9. Sensitivity Analysis for SSL Dilution Factor Model

Parameter assignments	Dilution Factor			Mixing depth (m)	
	Source area				
	30-acre	0.5-acre	Ratio of 0.5-acre/30-acre	30-acre	0.5 acre
All central parameters	5.2	15	2.9	12	5.1
Less conservative					
Darcy velocity	85	263	3.1	12	4.8
Aquifer thickness	15	15	1.0	40	5.1
Infiltration rate	39	118	3.0	12	4.8
More conservative					
Darcy velocity	1.2	2.1	1.8	12	12
Aquifer thickness	2.1	9.1	4.3	3.0	3.0
Infiltration rate	3.2	8.7	2.7	12	5.5

Input parameters	Conservatism		
	Less	Nominal	More
Darcy velocity (DV, m/yr)	442	22	0.8
Aquifer thickness (da, m)	46	12	3
Infiltration rate (m/yr)	0.02	0.18	0.35

Parameter sources

Percentile	DV[a] (m/yr)	da[b] (m)
10th	0.8	3.0
25th	4	5.5
50th	22	11
75th	121	23
90th	442	46
Average:	800	28
Geomean:	22	12

[a] 300 DNAPL & HGDB sites.

[b] 208 HGDB sites.

- Change the volatilization rate to a value corresponding to the uniform release of the total mass of contaminants over the period of exposure.

The latter approach was taken in the draft Risk-Based Corrective Action (RBCA) screening methodology developed by the American Society for Testing and Materials (ASTM) (ASTM, 1994). As stated on page B6 of the RBCA guidance (B.6.6.6):

> In the event that the time-averaged flux exceeds that which would occur if all chemicals initially present in the surficial soil zone volatilized during the exposure period, then the volatilization factor is determined from a mass balance assuming that all chemical initially present in the surficial soil zone volatilizes during the exposure period.

This was selected over the exposure duration option because it is reasonably conservative for screening purposes (obviously, more contaminant cannot possibly volatilize from the soil) and it avoided the uncertainties associated with applying the current models to estimate source depletion rates.

In summary, the mass-limit approach offers the following advantages:

- It corrects the possible mass-balance violation in the infinite-source SSLs.

- It does not require development of a finite source model to calculate SSLs.

- It is appropriate for screening, being based on the conservative assumption that all of the contaminant present leaches or volatilizes over the period of exposure.

- It is easy to develop and implement, requiring only very simple algebraic equations and input parameters that are, with the exception of source depth, already used to calculate SSLs.

The derivation of these models is described below. It should be noted that the American Industrial Health Council (AIHC) independently developed identical models to solve the mass-balance violation as part of their public comments on the Soil Screening Guidance.

2.6.2 Migration to Ground Water Mass-Limit Model. For the migration to ground water pathway, the mass of contaminant leached from a contaminant source over a fixed exposure duration (ED) period can be calculated as

$$M_l = C_w \times I \times A_s \times ED \qquad \textbf{(47)}$$

where

M_l = mass of contaminant leached (g)
C_w = leachate contaminant concentration (mg/L or g/m^3)
I = infiltration rate (m/yr)
A_s = source area (m^2)
ED = exposure duration (yr).

The total mass of contaminants present in a source can be expressed as

$$M_T = C_t \times \rho_b \times A_s \times d_s \tag{48}$$

where

M_T = total mass of contaminant present (g)
C_t = total soil contaminant concentration (mg/kg or g/Mg, dry basis)
ρ_b = dry soil bulk density (kg/L or Mg/m^3)
A_s = source area (m^2)
d_s = source depth (m).

To avoid a mass balance violation, the mass of contaminant leached cannot exceed the total mass of contaminants present (i.e., M_l cannot exceed M_T). Therefore, the maximum possible contaminant mass that can be leached from a source (assuming no volatilization or degradation) is M_T and the upper limit for M_l is

$$M_l = M_T$$

or

$$C_w \times I \times A_s \times ED = C_t \times \rho_b \times A_s \times d_s$$

Rearranging to solve for the total soil concentration (C_t) corresponding to this situation (i.e., maximum possible leaching)

Mass-Limit Model for Migration to Ground Water Pathway

$$C_t = (C_w \times I \times ED)/(\rho_b \times d_s) \tag{49}$$

Parameter/Definition (units)	Default
C_t/screening level in soil (mg/kg)	–
C_w/target soil leachate concentration (mg/L)	(nonzero MCLG, MCL, or HBL) × 20 DAF
I/infiltration rate (m/yr)	site-specific
ED/exposure duration (yr)	70
ρ_b/dry soil bulk density (kg/L)	1.5
d_s/average source depth (m)	site-specific

This soil concentration (C_t) represents a lower limit for soil screening levels calculated for the migration to ground water pathway. It represents the soil concentration corresponding to complete release of soil contaminants over the ED time period at a constant soil leachate concentration (C_w). Below this C_t, the soil leachate concentration averaged over the ED time period cannot exceed C_w.

2.6.3 Inhalation Mass-Limit Model. The volatilization factor (VF) is basically the ratio of the total soil contaminant concentration to the air contaminant concentration. VF can be calculated as

$$VF = (Q/C) \times (C_T^o/J_s^{ave}) \times 10^{-10}\ m^2kg/cm^2mg \qquad \textbf{(50)}$$

where

VF = volatilization factor (m^3/kg)
Q/C = inverse concentration factor for air dispersion (g/m^2-s per kg/m^3)
C_T^o = total soil contaminant concentration at t=0 (mg/kg or g/Mg, dry basis)
J_s^{ave} = average rate of contaminant flux from the soil to the air (g/cm^2-s).

The total amount of contaminant contained within a finite source can be written as

$$M_t = C_T^o \times \rho_b \times A_s \times d_s \qquad \textbf{(51)}$$

where

M_t = total mass of contaminant within the source (g)
C_T^o = total soil contaminant concentration at t=0 (mg/kg or g/Mg, dry basis)
ρ_b = soil dry bulk density (kg/L = Mg/m^3)
A_s = area of source (m^2)
d_s = depth of source (m).

If all of the contaminant contained within a finite source is volatilized over a given averaging time period, the average volatilization flux can be calculated as

$$J_s^{ave} = M_t/[(A_s \times 10^4\ cm^2/m^2) \times (T \times 3.15E7\ s/yr)] \qquad \textbf{(52)}$$

where

T = exposure period (yr).

Substituting Equation 51 for M_t in Equation 52 yields

$$J_s^{ave} = (C_T^o \times \rho_b \times d_s) / (10^4\ cm^2/m^2 \times T \times 3.15E7\ s/yr) \qquad \textbf{(53)}$$

Rearranging Equation 53 yields

$$C_T^o/J_s^{ave} = (10^4\ cm^2/m^2 \times T \times 3.15E7\ s/yr)/(\rho_b \times d_s) \qquad \textbf{(54)}$$

Substituting Equation 54 into Equation 50 yields

Mass-Limit Model for Inhalation of Volatiles

$$VF = (Q/C) \times [(T \times 3.15E7\ s/yr)/(\rho_b \times d_s \times 10^6\ g/Mg)] \qquad \textbf{(55)}$$

Parameter/Definition (units)	Default
VF/volatilization factor (m^3/kg)	–
Q/C/inverse of mean conc. at center of source (g/m^2-s per kg/m^3)	Table 3
T/exposure interval (yr)	30
ρ_b/dry soil bulk density (kg/L)	1.5
d_s/average source depth (m)	site-specific

If the VF calculated using an infinite source volatilization model for a given contaminant is less than the VF calculated using Equation 55, then the assumption of an infinite source may be too conservative for that specific contaminant at that source. Consequently, VF, as calculated in Equation 55, could be considered a minimum value for VF.

2.7 Plant Uptake

Commentors have raised concerns that the ingestion of contaminated produce from homegrown gardens may be a significant exposure pathway. EPA evaluated empirical data on plant uptake, particularly the data presented in the *Technical Support Document for Land Application of Sewage Sludge*, often referred to as the "Sludge Rule" (U.S. EPA, 1992d).

EPA found that empirical plant uptake-response slopes were available for selected metals but that available data were insufficient to estimate plant uptake of organics. In an effort to obtain additional empirical data, EPA has jointly funded research with the State of California on plant uptake of organic contaminants. These studies support ongoing revisions to the indirect, multimedia exposure model CalTOX.

The Sludge Rule identified six metals of concern with empirical plant uptake data: arsenic, cadmium, mercury, nickel, selenium, and zinc. Plant uptake-response slopes were given for seven plant categories such as grains and cereals, leafy vegetables, root vegetables, and garden fruits. EPA evaluated the study conditions (e.g., soil pH, application matrix) and methods (e.g., geometric mean, default values) used to calculate the plant uptake-response slopes for each plant category and determined that the geometric mean slopes were generally appropriate for calculating SSLs for the soil-plant-human exposure pathway.

However, the geometric mean of empirical uptake-response slopes from the Sludge Rule must be interpreted with caution for several reasons. First, the dynamics of sludge-bound metals may differ from the dynamics of metals at contaminated sites. For example, the empirical data were derived from a variety of studies at different soil conditions using different forms of the metal (i.e., salt vs. nonsalt). In studies where the application matrix was sludge, the adsorption power of sludge in the presence of calcium ions may have reduced the amount of metal that is bioavailable to plants and, therefore, plant uptake may be greater in non-sludge-amended soils.

In addition to these confounding conditions, default values of 0.001 were assigned for plant uptake in studies where the measured value was below 0.001. A default value was needed to calculate the geometric mean uptake-response slope values. Moreover, considerable study-to-study variability is shown in the plant uptake-response slope values (up to 3 orders of magnitude for certain plant/metal combinations). This variability could result from varying soil characteristics or experimental conditions, but models have not been developed to relate changes in plant uptake to such conditions. Thus, the geometric mean values represent "typical" values from the experiments; actual values at specific sites could show marked variation depending on soil composition, chemistry, and/or plant type.

OERR has used the information in the Sludge Rule to identify six metals (arsenic, cadmium, mercury, nickel, selenium, and zinc) of potential concern through the soil-plant-human exposure pathway for consideration on a site-specific basis. The fact that these metals have been identified should not be misinterpreted to mean that other contaminants are not of potential concern for this pathway. Other EPA offices are looking at empirical data and models for estimating plant uptake of organic contaminants from soils and OERR will incorporate plant uptake of organics once these efforts are reviewed and finalized.

Methods for evaluating the soil-plant-human pathway are presented in Appendix G. Generic screening levels are calculated based on the uptake factors (i.e., bioconcentration factors [Br]) presented in the Sludge Rule. Generic plant SSLs are compared with generic SSLs based on direct ingestion as well as levels of inorganics in soil that have been reported to cause phytotoxicity (Will and Suter, 1994). Although site-specific factors such as soil type, pH, plant type, and chemical form will determine the significance of this pathway, the results of our analysis suggest that the soil-plant-human pathway may be of particular concern for sites with soils contaminated with arsenic or cadmium. Likewise, the potential for phytotoxicity will be greatly influenced by site-specific factors; however, the data presented by Will and Suter (1994) suggest that, with the exception of arsenic, the levels of inorganics that are considered toxic to plants are well below the levels that may impact human health via the soil-plant-human pathway.

2.8 Intrusion of Volatiles into Basements: Johnson and Ettinger Model

Concern about the potential impact of contaminated soil on indoor air quality prompted EPA to consider the Johnson and Ettinger (1991) model, a heuristic model for estimating the intrusion rate of contaminant vapors from soil into buildings. The model is a closed-form analytical solution for both convective and diffusive transport of vapor-phase contaminants into enclosed structures located above the contaminated soil. The model may be solved for both steady-state (i.e., infinite source) or quasi-steady-state (i.e., finite source) conditions. The model incorporates a number of key assumptions, including no leaching of contaminant to ground water, no sinks in the building, and well-mixed air volume within the building.

To evaluate the effects of using the Johnson and Ettinger model on SSLs for volatile organic contaminants, EPA contracted Environmental Quality Management, Inc. (EQ), to construct a case example to estimate a high-end exposure point concentration for residential land use (Appendix H; EQ and Pechan, 1994). The case example models a contaminant source relatively close or directly beneath a building where the soil beneath the building is very permeable and the building is underpressurized, tending to pull contaminants into the basement. Where possible and appropriate, values of model variables were taken directly from Johnson and Ettinger (1991). Using both steady-state and quasi-steady-state formulations, building air concentrations of each of 42 volatile SSL chemicals were calculated. The inverses of these concentrations were substituted into the inhalation SSL equations (Equations 4 or 5) as an indoor volatilization factor (VF_{indoor}) to calculate carcinogenic or noncarcinogenic SSLs based on migration of contaminants into basements (i.e., "indoor inhalation" SSLs).

Results showed a difference of up to 2 orders of magnitude between the steady-state and quasi-steady-state results for the indoor inhalation SSLs. Infinite source indoor inhalation SSLs were less than the corresponding "outdoor" inhalation SSLs by as much as 3 orders of magnitude for highly volatile constituents. For low-volatility constituents, the difference was considerably less, with no difference in the indoor and outdoor SSLs in some cases. The EQ study also indicated that the most important input parameters affecting long-term building concentration (and thus the SSL) are building ventilation rate, distance from the source (i.e., source-building separation), soil permeability to vapor flow, and source depth. For lower-permeability soils, the number and size of cracks in the basement walls may be more significant, although this was not a significant variable for the permeable soils considered in the study.

EPA decided against using the Johnson and Ettinger model to calculate **generic** SSLs due to the sensitivity of the model to parameters that do not lend themselves to standardization on a national basis (e.g., source depth, the number and size of cracks in basement walls). In addition, the only formal validation study identified by EPA compares model results with measured radon concentrations from a highly permeable soil. Although these results compare favorably, it is not clear how applicable they are to less permeable soils and compounds not already present in soil as a gas (as radon is).

The model can be applied on a site-specific basis in conjunction with the results of a soil gas survey. Where land use is currently residential, a soil gas survey can be used to measure the vapor phase concentrations at the foundation of buildings, thereby eliminating the need to model partitioning of contaminants, migration from the source to the basement, and soil permeability.

For future use scenarios, although some site-specific data are available, the difficulties are similar to those encountered with generic application of the model. Predictions must be made regarding the distance from the source to the basement and the permeability of the soil, basement floor, and walls. EQ's report models the potential impact of placing a structure directly above the source. Depending on the permeability of the surrounding soils, the results suggest that the level of residual contamination would have to be extremely low to allow for such a scenario. Distance from the source can have a dramatic impact on the results and should be considered in more detailed investigations involving future residential use scenarios.

Part 3: MODELS FOR DETAILED ASSESSMENT

The Soil Screening Guidance addresses the inhalation and migration to ground water exposure pathways with simple equations that require a small number of easily obtained soil parameters, meteorologic conditions, and hydrogeologic parameters. These equations incorporate a number of conservative simplifying assumptions—an infinite source, no fractionation between pathways, no biological or chemical degradation, no adsorption—conditions that can be addressed with more complicated models. Applying such models will more accurately define the risk of exposure via the inhalation or the migration to ground water pathway and, depending on site conditions, can lead to higher SSLs that are still protective. However, input data requirements and modeling costs make this option more expensive to implement than the SSL equations.

This part of the Technical Background Document presents information on the selection and use of more complex fate and transport models for calculating SSLs. Generally, the decision to use these models will involve balancing costs: if the models and assumptions used to develop simple site-specific SSLs are overly conservative with respect to site conditions (e.g., a thick unsaturated zone), the additional cost and time required to apply these models may be offset by the potential cost savings associated with higher, but still protective, SSLs.

Sections 3.1 and 3.2 include information on equations and models that can accommodate finite contaminant sources and fractionate contaminants between pathways (e.g., VLEACH and EMSOFT) and predict the subsequent impact on either ambient air or ground water. However, when using a finite source model, the site manager should recognize the uncertainties inherent in site-specific estimates of subsurface contaminant distributions and use conservative estimates of source size and concentrations to allow for such uncertainties. In addition, model predictions should be validated against actual site conditions to the extent possible.

3.1 Inhalation of Volatiles: Detailed Models

Developing SSLs for the inhalation of volatiles involves calculating a site-specific volatilization factor (VF) and dispersion factor (Q/C). This section provides a brief description of finite source volatilization models with potential applicability to SSL development and information on site-specific application of the AREA-ST dispersion model for estimating the Q/C values needed to calculate both VF and PEF. It should not be viewed as an official endorsement of these models (other volatilization models may be available with applicability to SSL development).

3.1.1 Finite Source Volatilization Models. To identify suitable models for addressing a finite contaminant source, EPA contracted Environmental Quality Management, Inc. (EQ), to conduct a preliminary evaluation of a number of soil volatilization models, including volatilization models developed by Hwang and Falco (1986), as modified by EQ (1992), and by Jury et al. (1983, 1984, and 1990) and VLEACH, a multipathway model developed primarily to assess exposure through the ground water pathway. Study results (EQ and Pechan, 1994) show reasonable agreement (within a factor of 2) between emission predictions using the modified Hwang and Falco or Jury models, but consistently lower predictions from VLEACH. However, Shan and Stephens (1995) discovered an error in the VLEACH calculation of the apparent diffusivity, which has been subsequently corrected. The corrected VLEACH model, version 2.2, appears to provide emission estimates similar to the Jury and the modified Hwang and Falco models. The revised VLEACH (v.2.2) program is available from the Center for Subsurface Modeling Support (CSMOS) at EPA's Environmental Research Laboratory in Ada, Oklahoma (WWW.EPA.GOV/ADA/ CSMOS.HTML), and is discussed further in Section 3.2.

For certain contaminant conditions, Jury et al. (1990) present a simplified equation (Jury's Equation B1) for estimating the flux of a contaminant from a finite source of contaminated soil. The following assumptions were used to derive this simplified flux equation:

- Uniform soil properties (e.g., homogeneous average soil water content, bulk density, porosity, and fraction organic carbon)
- Instantaneous linear equilibrium adsorption
- Linear equilibrium liquid-vapor partitioning (Henry's law)
- Uniform initial contaminant incorporation at t=0
- Chemicals in a dissolved form only (i.e., soil contaminant concentrations are below C_{sat})
- No boundary layer thickness at ground level (no stagnant air layer)
- No water evaporation or leaching
- No chemical reactions, biodegradation, or photolysis
- $d_s >> (4D_At)^{1/2}$ (ramifications of this are discussed below).

Under these assumptions, the Jury et al. (1990) simplified finite source model is

$$J_s = C_o(D_A/\pi t)^{1/2}[1-\exp(-d_s^2/4D_At)] \qquad \textbf{(56)}$$

where

J_s = contaminant flux at ground surface (g/cm^2-s)
C_o = uniform contaminant concentration at t=0 (g/cm^3)
D_A = apparent diffusivity (cm^2/s)
π = 3.14
t = time (s)
d_s = depth of uniform soil contamination at t=0 (cm),

and

$$D_A = [(\theta_a^{10/3} D_i H' + \theta_w^{10/3} D_w)/n^2]/(\rho_b K_d + \theta_w + \theta_a H') \qquad \textbf{(57)}$$

where

θ_a = air-filled soil porosity (L_{air}/L_{soil}) = $n - \theta_w$
n = total soil porosity (L_{pore}/L_{soil}) = $1 - (\rho_b/\rho_s)$
θ_w = water-filled soil porosity (L_{water}/L_{soil}) = $w\rho_b/\rho_w$
ρ_b = soil dry bulk density (g/cm^3)
ρ_s = soil particle density (g/cm^3)
w = average soil moisture content (g/g)

ρ_w = water density (g/cm^3)
D_i = diffusivity in air (cm^2/s)
H' = dimensionless Henry's law constant = 41 × HLC
HLC = Henry's law constant (atm-m^3/mol)
D_w = diffusivity in water (cm^2/s)
K_d = soil-water partition coefficient (cm^3/g) = K_{oc} f_{oc}
K_{oc} = soil organic carbon partition coefficient (cm^3/g)
f_{oc} = organic carbon content of soil (g/g).

To estimate the average contaminant flux over 30 years, the time-dependent contaminant flux **must be solved for various times and the results averaged**. A simple computer program or spreadsheet can be used to calculate the instantaneous flux of contaminants at set intervals and numerically integrate the results to estimate the average contaminant flux. However, the time-step interval must be small enough (e.g., 1-day intervals) to ensure that the cumulative loss through volatilization is less than the total initial mass. Inadequate time steps can lead to mass-balance violations.

To address this problem, EPA/ORD's National Center for Environmental Assessment has developed a computer modeling program, EMSOFT. The computer program provides an average emission flux over time by using an analytical solution to the integral, thereby eliminating the problem of establishing adequate time steps for numerical integration. In addition, the EMSOFT model can account for water convection (i.e., leaching), and the impact of a soil-air boundary layer on the flux of contaminants with low Henry's law constants. EMSOFT will be available through EPA's National Center for Environmental Assessment (NCEA) in Washington, DC.

Once the average contaminant flux is calculated, VF is calculated as:

$$VF = (Q/C) \times (C_o/\rho_b) \times (1/J_s^{ave}) \times 10^{-4}\ m^2/cm^2 \qquad \textbf{(58)}$$

where

VF = volatilization factor (m^3/kg)
Q/C = inverse concentration factor for air dispersion (g/m^2-s per kg/m^3)
C_o = uniform contaminant concentration at t=0 (g/cm^3)
ρ_b = soil dry bulk density (g/cm^3)
J_s^{ave} = average rate of contaminant flux (g/cm^2-s).

3.1.2 Air Dispersion Models. The inverse concentration factor for air dispersion, Q/C, is used in the determination of both VF and PEF. For a detailed site-specific assessment of the inhalation pathway, a site-specific Q/C can be determined using the Industrial Source Complex Model platform in the short-term mode (ISCST3). Only a very brief overview of the application, assumptions, and input requirements for the model as used to determine Q/C is provided in this section. This model is the final regulatory version of the ISCST3 model.

The ISCST3 model FORTRAN code, executable versions, sample input and output files, description, and documentation can be downloaded from the "Other Models" section of the Office of Air Quality Planning and Standards (OAQPS) Support Center for Regulatory Air Models bulletin board system (SCRAM BBS). To access information, call:

OAQPS SCRAM BBS
(919) 541-5742 (24 hours/day, 7 days/week except Monday AM)
1,200–9,600, 14,400 baud
Line Settings: 8 bits, no parity, 1 stop bit
Terminal Emulation: VT100 or ANSI
System Operator: (919) 541-5384 (normal business hours EST).

The user registers in the first call and then has full access to the BBS.

The ISCST3 model will output an air concentration (in $\mu g/m^3$) when the concentration model option is selected (e.g., CO MODELOPT DFAULT CONC rural/urban). The surface area of the contaminated soil source must be determined. For the ISCST3 model, the source location of an area source is defined by the coordinates of the southwest corner of the square (e.g., SO LOCATION sourcename AREA $-^1/_2$length $-^1/_2$width height=0). For the source parameter input line, the contaminant's area emission rate (in units of g/m^2-s) must be entered. The area emission rate is the site-specific average emission flux rate, as calculated in Equation 56, converted to units of g/m^2-s (i.e., Aremis = $J_s^{ave} \times 10^4\ cm^2/m^2$). Alternatively, an area emission rate of 1 g/m^2-s can be assumed. A grid or circular series of receptor sites should be used in and around the area source to identify the point of maximum contaminant air concentration. Hourly meteorologic data (*.MET files) for the nearest city (i.e., airport) of similar terrain and the preprocessor PCRAMMET also can be downloaded from the SCRAM BBS.

The ISCST3 model output concentration is then used to calculate Q/C as

$$Q/C = (J_s^{ave} \times 10^4\ cm^2/m^2)/(C_{air} \times 10^{-9}\ kg/\mu g) \qquad \textbf{(59)}$$

where

Q/C = inverse concentration factor for air dispersion (g/m^2-s per kg/m^3)
J_s^{ave} = average rate of contaminant flux (g/cm^2-s)
C_{air} = ISC output maximum contaminant air concentration ($\mu g/m^3$).

Note: If an area emission rate of 1 g/m^2-s is assumed, then ($J_s^{ave} \times 10^4\ cm^2/m^2$) = 1, and Equation 59 simplifies to simply the inverse of the maximum contaminant air concentration (in kg/m^3).

3.2 Migration to Ground Water Pathway

For the migration to ground water pathway, the SSL equations assume an infinite source, contamination extending to the water table, and no attenuation due to degradation or adsorption in the unsaturated zone. At sites with small sources, deep water tables, confining layers in the unsaturated zone that can block contaminant transport, or contaminants that degrade through biological or chemical mechanisms, more complex models that can address such site conditions can be used to calculate higher SSLs that still will be protective of ground water quality. This section provides information on the use of such models in the soil screening process to calculate a dilution-attenuation factor (Section 3.2.1) and to estimate contaminant release in leachate and transport through the unsaturated zone (Section 3.2.2).

3.2.1 Saturated Zone Models. EPA has developed guidance for the selection and application of saturated zone transport and fate models and for interpretation of model applications. The user is referred to *Ground Water Modeling Compendium, Second Edition 1994* (U.S. EPA, 1994b) and *Framework for Assessing Ground Water Modeling Applications* (U.S. EPA, 1994a) for further information.

More complex saturated zone models can be used to calculate a dilution-attenuation factor (DAF) that, unlike the SSL dilution model, can consider attenuation in the aquifer. Some can handle a finite source through a transient mode that requires a time-stepped concentration from a finite-source unsaturated zone model (see Section 3.2.2). In general, to calculate a DAF using such models, the contaminant concentration at the water table under the source (C_w) is set to unity (e.g., 1 mg/L). The DAF is the reciprocal of the predicted concentration at the receptor point (C_{RP}) as follows:

$$DAF = C_w / C_{RP} = 1/C_{RP} \tag{60}$$

3.2.2 Unsaturated Zone Models. In an effort to provide useful information for model application, EPA's ORD laboratories in Ada, Oklahoma, and Athens, Georgia, conducted an evaluation of nine unsaturated zone fate and transport models (Criscenti et al., 1994; Nofziger et al., 1994). The results of this effort are summarized here. The models reviewed are only a subset of the potentially appropriate models available to the public and are not meant to be construed as having received EPA approval. Other models also may be applicable to SSL development, depending on site-specific circumstances.

Each of the unsaturated zone models selected for evaluation are capable, to varying degrees, of simulating the transport and transformation of chemicals in the subsurface. Even the most unique site conditions can be simulated by either a single model or a combination of models. However, the intended uses and the required input parameters of these models vary. The models evaluated include:

- RITZ (Regulatory and Investigative Treatment Zone model)
- VIP (Vadose zone Interactive Process model)
- CMLS (Chemical Movement in Layered Soils model)
- HYDRUS
- SUMMERS (named after author)
- MULTIMED (MULTIMEDia exposure assessment model)
- VLEACH (Vadose zone LEACHing model)
- SESOIL (SEasonal SOIL compartment model)
- PRZM-2 (Pesticide Root Zone Model).

RITZ, VIP, CMLS, and HYDRUS were evaluated by Nofziger et al. (1994). SUMMERS, MULTIMED, VLEACH, SESOIL, and PRZM-2 were evaluated by Criscenti et al. (1994). These documents should be consulted for further information on model application and use.

The applications, assumptions, and input requirements for the nine models evaluated are described in this section. The model descriptions include model solution method (i.e., analytical, numerical), the purpose of the model, and descriptions of the methods used by the model to simulate water/contaminant transport and contaminant transformation. Each description is accompanied by a table of required input parameters. Input parameters discussed include soil properties, chemical properties, meteorologic data, and other site information. In addition, certain input control parameters may be required such as time stepping, grid discretization information, and output format.

Information on determining general applicability of the models to subsurface conditions is provided, followed by an assessment of each model's potential applicability to the soil screening process.

RITZ. Information on the RITZ model was obtained primarily from Nofziger et al. (1994). RITZ is a steady-state analytical model used to simulate the transport and fate of chemicals mixed with oily wastes (sludge) and disposed of by land treatment. RITZ simulates two layers of the soil column with uniform properties. The soil layers consist of: (1) the upper plow zone where the oily waste is applied and (2) the treatment zone. The bottom of the treatment zone is the water table. It is assumed in the model that the oily waste is completely mixed in and does not migrate out of the plow zone, which represents the contaminant source at an initial time. RITZ also assumes an infinite source (i.e., a continuous flux at constant concentration). The flux of water is assumed to be constant with time and depth and the Clapp-Hornberger constant is used in defining the soil water content resulting from a specified recharge rate. Sorption, vapor transport, volatilization, and biochemical degradation are also considered (van der Heijde, 1994). Partitioning between phases is instantaneous, linear, and reversible. Input parameters required for the RITZ model are presented in Table 10. Biochemical degradation of the oil and contaminant is considered to be a first-order process, and dispersion in the water phase is ignored.

Table 10. Input Parameters Required for RITZ Model

Soil properties	Site characteristics	Pollutant properties	Oil properties
Percent organic carbon	Plow zone depth	Concentration in sludge	Concentration of oil in sludge
Bulk density	Treatment zone depth	K_{oc}	Density of oil
Saturated water content	Recharge rate (constant)	K_{ow}	Degradation half-life of oil
Saturated hydraulic conductivity	Evaporation rate (constant)	Henry's law constant	---
Clapp-Hornberger constant	Air temperature (constant)	Degradation half-life (constant)	---
---	Relative humidity (constant)	Diffusion coefficient (in air)	---
---	Sludge application rate	---	---
---	Diffusion coefficient (water vapor in oil)	---	---

VIP. Information on the VIP model was obtained from Nofziger et al. (1994). The VIP model is a one-dimensional, numerical (finite-difference) fate and transport model also designed for simulating the movement of compounds in the unsaturated zone resulting from land application of oily wastes. Like the RITZ model, VIP considers dual soil zones (a plow zone and a treatment zone) and considers the source to be infinite. VIP differs from RITZ in that it solves the governing differential equations numerically, which allows variability in the flux of water and chemicals over time. Advection and hydrodynamic dispersion are the primary transport mechanisms for the contaminant in water (van der Heijde, 1994). Instead of assuming instantaneous, linear equilibrium between all phases, VIP considers the partitioning rates between the air, oil, soil, water, and vapor-phase transport. Contaminant transformation processes include hydrolysis, volatilization, and sorption. Oxygen-limited degradation and diffusion of the contaminant in the air phases are also considered. Sorption is instantaneous as described for the RITZ model. The input parameters required for the VIP model are presented in Table 11.

Table 11. Input Parameters Required for VIP Model

Soil properties	Site characteristics	Pollutant properties	Oxygen properties	Oil properties
Porosity	Plow zone depth	Concentration in sludge	Oil-air partition coefficient[a]	Density of oil
Bulk density	Treatment zone depth	Oil-water partition coefficient[a]	Water-air partition coefficient[a]	Degradation rate constant of oil
Saturated hydraulic conductivity	Mean daily recharge rate	Air-water partition coefficient[a]	Oxygen half-saturation constant in air phase [a]	---
Clapp-Hornberger constant	Temperature (each layer)	Soil-water partition coefficient[a]	Oxygen half-saturation constant in oil phase [a]	---
---	Sludge application rate	Degradation constant in oil[a]	Oxygen half-saturation constant in water phase[a]	---
---	Sludge density	Degradation constant in water[a]	Oxygen half-saturation constant (oil degradation)	---
---	Application period and frequency in period	Dispersion coefficient	Stoichiometric ratio of oxygen to pollutant consumed	---
---	Weight fraction water in sludge	Adsorption-desorption rate constant (water/oil)	Stoichiometric ratio of oxygen to oil consumed	---
---	Weight fraction oil in waste	Adsorption-desorption rate constant (water/soil)	Oxygen transfer rate coefficient between oil and air phases	---
---	---	Adsorption-desorption rate constant (water/air)	Oxygen transfer rate coefficient between water and air phases	---

[a] Parameters required for plow zone and treatment zone.

CMLS. Information on CMLS was obtained from Nofziger et al. (1994). CMLS is an analytical model developed as a management tool to describe the fate and transport of pesticides in layered soils and to estimate the amount of chemical at a certain position at a certain time. The model allows designation of up to 20 soil layers with uniform soil and chemical properties defined for each layer.

Water in the soil system is "pushed ahead" of new water (recharge) entering the system. The water content is reduced to the field capacity after each infiltration event, and water is removed from the root zone in proportion to the available water stored in that layer (Nofziger et al., 1994). CMLS assumes movement of the chemical in liquid phase only and allows a finite source. Chemical partitioning between the soil and the water is assumed to be linear, instantaneous, and reversible. Volatilization is not considered. Dispersion and diffusion of the chemical is ignored and degradation is defined as a first-order process. The input parameters required for the CMLS model are presented in Table 12.

Table 12. Input Parameters Required for CMLS

Soil properties	Site characteristics	Chemical properties
Depth of bottom of soil layers	Daily infiltration or precipitation	Degradation half-life (each soil layer)
Organic carbon content	Daily evapotranspiration	Amount applied
Bulk density	---	Depth of application
Saturated water content	---	Date of application
Field capacity	---	K_{oc}
Permanent wilting point	---	---

HYDRUS. Information on the HYDRUS model was obtained from Nofziger et al. (1994). HYDRUS is a finite-element model for one-dimensional solute fate and transport simulations. The boundary conditions for flow, as well as soil and chemical properties, can therefore vary with time. A finite source also can be modeled. Soil parameters are described by the van Genuchten parameters. The model also considers root uptake and hysteresis in the water movement properties. Solute transport and transformation incorporates molecular diffusion, hydrodynamic dispersion, linear or nonlinear equilibrium partitioning (sorption), and first-order decay (van der Heijde, 1994). Volatilization is not considered. The input parameters required by HYDRUS are presented in Table 13.

SUMMERS. Information on the SUMMERS model was obtained from Criscenti et al. (1994). SUMMERS is a one-dimensional analytical model that simulates one-dimensional, nondispersive transport in a single layer of soil from an infinite source. It was developed to determine the contaminant concentrations in soil that would result in ground water contamination above specified levels for evaluating geothermal energy sites. The model is similar to the SSL equations in that it assumes steady-state water movement and equilibrium partitioning of the contaminant in the unsaturated zone and performs a mass-balance calculation of mixing in an underlying aquifer. For the saturated zone, the model assumes a constant flux from the surface source and instantaneous, complete mixing in the aquifer. The mixing depth is therefore defined by the thickness of the aquifer. The model does not account for volatilization. The input parameters required for SUMMERS are listed in Table 14.

Table 13. Input Parameters Required for HYDRUS

Soil properties	Site characteristics	Pollutant properties	Root uptake parameters
Depth of soil layers	Uniform or stepwise rainfall intensity	Molecular diffusion coefficient	Power function in stress-response function
Saturated water content	Contaminant concentrations in soil	Dispersivity	Pressure head where transpiration is reduced by 50%
Saturated hydraulic conductivity	---	Decay coefficient (dissolved)	Root density as a function of depth
Bulk density	---	Decay coefficient (adsorbed)	---
Retention parameters	---	Freundlich isotherm coefficients	---
Residual water content	---	---	---

Table 14. Input Parameters Required for SUMMERS

Parameters required	
Target concentration in ground water	Thickness of aquifer
Volumetric infiltration rate into aquifer	Width of pond/spill perpendicular to flow
Downward porewater velocity	Initial (background) concentration
Ground water seepage velocity	Equilibrium partition coefficient
Void fraction	Darcy velocity in aquifer
Horizontal area of pond or spill	Volumetric ground water flow rate

MULTIMED. Information on the MULTIMED model was obtained from Criscenti et al. (1994) and Salhotra et al. (1990). MULTIMED was developed as a multimedia fate and transport model to simulate contaminant migration from a waste disposal unit. For this review, only the fate and transport of pollutants from the soil to migration to ground water pathway was considered in detail.

In MULTIMED, infiltration of waste into the unsaturated or saturated zones can be simulated using a landfill module or by direct infiltration to the unsaturated or saturated zones. Flow in the unsaturated zone and for the landfill module is simulated by a one-dimensional, semianalytical module. Transport in the unsaturated zone considers the effects of dispersion, sorption, volatilization, biodegradation, and first-order chemical decay. The saturated transport module is also one-dimensional, but considers three-dimensional dispersion, linear adsorption, first-order decay, and dilution due to recharge. Mixing in the underlying saturated zone is based on the vertical dispersivity specified, the length of the disposal facility parallel to the flow direction, the thickness of the saturated zone, the ground water velocity, and the infiltration rate. The saturated zone module can simulate steady-state and transient ground water flow and thus can consider a finite source assumption through a leachate "pulse duration." The parameters required for the unsaturated and saturated zone transport in MULTIMED are presented in Table 15.

Table 15. Input Parameters Required for MULTIMED

Unsaturated zone parameters		
Saturated hydraulic conductivity	Thickness of each layer	Reference temperature for air diffusion
Porosity	Longitudinal dispersivity	Molecular weight
Air entry pressure head	Percent organic matter	Infiltration rate
Depth of unsaturated zone	Soil bulk density	Area of waste disposal unit
Residual water content	Biological decay coefficient	Duration of pulse
Number of porous materials	Acid, base, and neutral hydrolysis rates	Source decay constant
Number of layers	Reference temperature	Initial concentration at landfill
Alpha coefficient	Normalized distribution coefficient	Particle diameter
van Genuchten exponent	Air diffusion coefficient	---
Saturated zone parameters		
Recharge rate	Longitudinal dispersivity	Organic carbon content
First-order decay coefficient	Transverse dispersivity	Well distance from site
Biodegradation coefficient	Vertical dispersivity	Angle off-center of well
Aquifer thickness	Temperature of aquifer	Well vertical distance
Hydraulic gradient	pH	---

VLEACH. Information on the VLEACH model was obtained from Criscenti et al. (1994). VLEACH is a one-dimensional, finite difference model developed to simulate the transport of contaminants displaying linear partitioning behavior through the vadose zone to the water table by aqueous advection and diffusion. Multiple layers can be modeled and are expressed as polygons with different soil properties and recharge rates. Water flow is assumed to be steady state. Linear equilibrium partitioning is used to determine chemical concentrations between the aqueous, gaseous, and adsorbed phases (sorption and volatilization), and a finite source can be considered. Chemical or biological degradation is not considered. The input parameters required for VLEACH are presented in Table 16.

Table 16. Input Parameters Required for VLEACH

Soil properties	Chemical characteristics	Site properties
Dry bulk density	K_{oc}	Recharge rate
Total porosity	Henry's law constant	Contaminant concentrations in recharge
Volumetric water content	Aqueous solubility	Depth to ground water
Fractional organic carbon	Free air diffusion coefficient	Dimensions of "polygons"

SESOIL. Information on the SESOIL model was obtained from Criscenti et al. (1994). SESOIL is a one-dimensional, finite difference flow and transport model developed for evaluating the movement of contaminants through the vadose zone. The model contains three components: (1) hydrologic cycle, (2) sediment cycle, and (3) pollutant fate cycle. The model estimates the rate of vertical solute transport and transformation from the land surface to the water table. Up to four layers can be simulated by the model and each layer can be subdivided into 10 compartments with uniform soil characteristics. Hydrologic data can be included using either monthly or annual data options. Solute transport is simulated for ground water and surface runoff including eroded sediment. Pollutant fate considers equilibrium partitioning to soil and air phases (sorption and diffusion), volatilization from the surface layer, first-order chemical degradation, biodegradation, cation exchange, hydrolysis, and metal complexation and allows for a stationary free phase. The required input parameters for SESOIL are presented in Table 17 for the monthly option.

Table 17. Input Parameters Required for SESOIL (Monthly Option)

Climate data	Soil data	Chemical data	Application data
Mean air temperature[a]	Number of layers and sublayers	Solubility in water	Application area
Mean cloud cover fraction[a]	Thickness of layers	Air diffusion coefficient	Site latitude
Mean relative humidity[a]	pH of each layer	Henry's law constant	Spill index
Short wave albedo fraction[a]	Bulk density	Organic carbon adsorption ratio	Pollutant load
Total precipitation	Intrinsic permeability	Soil adsorption coefficient	Mass removed or transformed
Mean storm duration	Pore disconnectedness index	Molecular weight	Index of volatile diffusion
Number of storm events	Effective porosity	Valence	Index of transport in surface runoff
—	Organic carbon content	Hydrolysis constants (acid, base, neutral)	Ratio pollutant conc. in rain to solubility
—	Cation exchange capacity	Biodegradation rates (liquid, solid)	Washload area
—	Freundlich exponent	Ligand stability constant	Average slope and slope length
—	Silt, sand, and clay fractions	Moles ligand per mole compound	Erodibility factor
—	Soil loss ratio	Molecular weight of ligand	Practice factor
—	—	Ligand mass	Manning coefficient

[a] SESOIL uses these parameters to calculate evapotranspiration if an evapotranspiration value is not specified.

PRZM-2. Information on PRZM-2 was obtained from Criscenti et al. (1994). PRZM-2 is a combination of two models developed to simulate the one-dimensional movement of chemicals in the unsaturated and saturated zones. The first model, PRZM, is a finite difference model that simulates water flow and detailed pesticide fate and transformation in the unsaturated zone. The second model, VADOFT, is a one-dimensional finite element model with more detailed water movement simulation capabilities. The coupling of these models results in a detailed representation of contaminant transport and transformation in the unsaturated zone.

PRZM has been used predominantly for evaluation of pesticide leaching in the root zone. PRZM uses detailed meteorologic and surface hydrology data for the hydrologic simulations. Runoff, erosion, plant uptake, leaching, decay, foliar washoff, and volatilization are considered in the surface hydrologic and chemical transport components. Chemical transport and fate in the subsurface is simulated by advection, dispersion, molecular diffusion, first-order chemical decay, biodegradation, daughter compound progeny, and soil sorption. The input parameters required for PRZM are presented in Table 18.

VADOFT can be run independently of PRZM and output from the PRZM model can be used to set the boundary conditions for VADOFT. The lower boundaries could also be specified as a constant pressure head or zero velocity. Transport simulations consider advection and diffusion with sorption and first-order decay. The input requirements for VADOFT are presented in Table 19.

Considerations for Unsaturated Zone Model Selection. The accuracy of a model in a site-specific application depends on simplifications and assumptions implicit in the model and their relationship to site-specific conditions. Additional error may be introduced from assumptions made when deriving input parameters. Although each of the nine models evaluated has been tested and validated for simulation of water and contaminant movement in the unsaturated zone, they are different in purpose and complexity, with certain models designed to simulate very specific scenarios.

A model should be selected to accommodate a site-specific scenario as closely as possible. For example, if contaminant volatilization is of concern, the model should consider volatilization and vapor phase transport. After a model is determined to be appropriate for a site, contaminant(s), and conditions to be modeled, the site-specific information available (or potentially available) should be compared to the input requirements for the model to ensure that adequate inputs can be developed.

The unsaturated zone models addressed in this study use either analytical, semianalytical, or numerical solution methods. Analytical models represent the simplest models, requiring the least number of input parameters. They use a closed-form solution for the pertinent equations. In analytical models, certain assumptions have to be made with respect to the geometry of the system and external stresses. For this reason, there are few analytical flow models (van der Heijde, 1994). Analytical solutions are common, however, for fate and transport problems by solution of convection-dispersion equations. Analytical models require the assumption of uniform flow conditions, both spatially and temporally.

Semianalytical models approximate complex analytical solutions using numerical techniques (van der Heijde, 1994). Transient or steady-state conditions can be approximated using a semianalytical model. However, spatial variability in soil or aquifer conditions cannot be accommodated.

Numerical models use approximations of pertinent partial differential equations usually by finite-difference or finite-element methods. The resolution of the area and time of simulation is defined by the modeler. Numerical models may be used when simulating time-dependent scenarios, spatially variable soil conditions, and unsteady flow (van der Heijde, 1994).

Table 18. Input Parameters Required for PRZM

Daily climate data			
Pan evaporation and pan factor	Precipitation	Windspeed	Snowmelt factor
Temperature	Monthly daylight hours	Solar radiation	Minimum evaporation extraction depth
Erosion data			
Topographic factor/soil erodibility	Average duration of rainfall	Field area	Practice factor
Crop data			
Surface condition of crop	Maximum interception storage	Maximum rooting depth	Maximum canopy coverage
Maximum dry weight of crop after harvest	---	Emergence, maturation, and harvest dates	---
Pesticide data			
Application quantity	Number of applications (50 maximum)	Number of chemicals (3 maximum)	Application dates
Foliar extraction coefficient	Incorporation depth	Plant uptake factor	Foliar decay rates
Diffusion coefficient in air	Enthalpy of vaporization	K_d and K_{oc}	Henry's law constant
Initial concentration levels	Parent/daughter transform rates	Aqueous, sorbed, vapor decay rates	
Soil data			
Compartment thicknesses	Runoff curve numbers	Core depth	Number and thickness of horizons
Soil drainage parameter	Hydrodynamic dispersion	Bulk density	Initial soil water content
Wilting point	Percent organic carbon	Field capacity	---
Soil temperature			
Heat capacity per unit volume	Albedo	Reflectivity of soil surface	Height of windspeed measurement
Thermal conductivity of horizon	Avgerage monthly bottom boundary temperature	Initial horizon temperature	Sand and clay content
Biodegradation and irrigation parameters (not presented)			

Table 19. Input Parameters Required for VADOFT

Pesticide data	Soil data	
Number of chemicals	Number of soil horizons	Relative permeability vs. saturation
Aqueous decay rate	Horizon thicknesses	Pressure head vs. saturation
Initial concentration	Saturated hydraulic conductivity	Residual water phase saturation
Longitudinal dispersivity	Effective porosity	Brooks and Corey n
Retardation coefficient	Air entry pressure head	van Genuchten alpha
Molecular diffusion	---	---
Conc. flux at first node (if independent of PRZM)	Input flux or head at first node (if independent of PRZM)	

In certain cases, input parameters to be used in a model are not definitively known. Some models allow some input parameters to be expressed as probability distributions rather than a single value, referred to as Monte Carlo simulations. This method can provide an estimate of the uncertainty of the model output (i.e., percent probability that a contaminant will be greater than a certain concentration at a depth), but requires knowledge of the parameter distributions. Alternatively, a bounding approach can be used to estimate the effects of likely parameter ranges on model results where there is uncertainty in input parameter values.

Model Applicability to SSLs. The unsaturated models evaluated herein can provide inputs necessary for soil screening by calculating leachate concentrations at the water table or by calculating infiltration rates. In the former application, they produce results comparable to the leach test option. As with the leach test, the leachate concentration from the model is **divided** by the dilution factor to obtain an estimated ground water concentration at the receptor well. This receptor point concentration is then compared with the acceptable ground water concentration to determine if a site's soils exceed SSLs.

Table 20 summarizes characteristics and capabilities of the models evaluated for this study. All nine of the models can calculate contaminant concentrations in leachate that has infiltrated down to the water table from the vadose zone, although CMLS requires a separate calculation to estimate leachate concentration. If there is reliable site data indicating significant degradation in soil, several of the models can consider biological and/or chemical degradation processes. The models also can address contaminant adsorption; those that can model layered soils can be especially useful in settings where low-permeability clay layers may attenuate contaminants through adsorption. Finally, several of the models can address a finite source if the size of the source is accurately known.

The average annual infiltration rate at a site is difficult to measure in the field yet is required for estimating a dilution factor or DAF. Four of the models evaluated, CMLS, HYDRUS, SESOIL, and PRZM, can calculate infiltration rates given either daily or monthly rainfall data.

Two models, VLEACH and SESOIL, address volatilization from the soil surface along with leachate emissions and therefore may be useful for SSL development for the volatilization and migration to ground water pathways. The volatile emission portion of VLEACH is discussed in Section 3.1.

Table 20. Characteristics of Unsaturated Zone Models Evaluated

	Type			Fate and Transport Processes Considered														Other		
Model	Analytical	Semianalytical	Numerical	Finite source	Partitioning with oil phase	Volatilization	Vapor phase transport	Hydrodynamic dispersion	Diffusion	Sorption	Nonequilibrium partitioning	Hydrolysis (1st-order decay)	Biodegradation	Layered soils	Root zone uptake	Runoff	Erosion	Saturated zone included	Monte Carlo analysis	Water balance calculations
RITZ	•				•	•			•	•		•	•							
VIP			•		•	•	•	•		•	•	•								
CMLS	•			•						•		•		•						•
HYDRUS			•	•				•	•	•		•		•	•					•
MULTIMED		•				•		•		•	•	•	•	•				•	•	
SUMMERS	•									•								•		
PRZM-2			•	•		•		•	•	•		•	•	•	•	•	•		•	•
SESOIL			•	•		•		•	•	•	•	•	•	•		•	•			•
VLEACH			•	•		•	•		•	•	•			•						

Table 20 addresses only unsaturated zone fate and transport model components, although two models (MULTIMED and SUMMERS) have saturated zone flow and transport capabilities. The following text highlights some of the differences between the models, outlines their advantages and disadvantages, and describes appropriate scenarios for model application.

RITZ. RITZ was designed to model land treatment units and is appropriate for sites where oily wastes are present (it includes sorption on an immobile oil phase as well as onto soil particles). Sorption, degradation, volatilization, and first-order decay processes are considered in the subsurface simulations. The most significant drawback for the model is the limit on the number of soil layers. Optimally, RITZ would be recommended for modeling chemical migration in a uniform unsaturated zone as a result of land application. Although the oil phase can be omitted for simulations of scenarios without oily materials, the RITZ model's focus on oily waste degradation in land treatment units limits its utility for soil screening (SSLs are not applicable when soils contain a separate oil phase).

VIP. VIP also is appropriate for sites where release of oily wastes has occurred. Some of the limitations described in RITZ also apply to the VIP model. VIP could be used as a followup model to RITZ since variable chemical and water fluxes can be simulated. In this case, significant additional input parameters are required to simulate transient partitioning between the air, soil, water, and oil phases. Like RITZ, VIP's focus on land treatment of oily waste limits its application to SSLs.

CMLS. CMLS differs from RITZ and VIP in that it allows designation of up to 20 soil layers with different properties. It does not consider nonaqueous phase liquids, dispersion, diffusion, or vapor phase transport, but a finite source can be modeled. CMLS estimates the location of the peak concentration of contaminants through a layered soil system. A limitation of the CMLS model for SSL application is that it does not calculate leachate concentrations. Instead, it calculates the amount of chemical at a certain depth at a certain time. The user must estimate the concentration based on the amount of chemical present and the total flux of water in the system (Nofziger et al., 1994). The model is typically used to estimate the time for a chemical entering the unsaturated zone to reach a certain depth.

HYDRUS. Like CMLS, the HYDRUS model can also simulate chemical movement in layered soils and can consider a finite source, but also includes dispersion and diffusion as well as sorption and first-order decay. In addition, HYDRUS outputs the chemical concentration in the soil water as a function of time and depth along with the amount of chemical remaining in the soil. The model considers root zone uptake, but other models such as PRZM should be used if the comprehensive effects of plant uptake are to be considered in the simulations. Because it can estimate infiltration from rainfall contaminant concentrations, HYDRUS may be useful in SSL applications.

SUMMERS. The SUMMERS model is a relatively simple model designed to simulate leaching in the unsaturated zone and is essentially identical to the SSL migration to ground water equations in assumptions and limitations. It is appropriate for use as an initial screening model where site data are limited and where volatilization is not of concern. However, since attenuation processes such as biodegradation, first-order decay, volatilization, or other attenuation processes (other than sorption) are not considered, it is a quite conservative model. Since volatilization is not considered, it cannot be used to simulate migration of volatile compounds to the atmosphere. Because of its similarities to the SSL migration to ground water equations, the SUMMERS model is not suitable for a more detailed assessment of site conditions.

MULTIMED. MULTIMED simulates simple vertical water movement in the unsaturated zone. Since an initial soil concentration cannot be specified, either the soil/water partition equation or a leaching test (SPLP) must be used to estimate soil leachate contaminant concentrations. MULTIMED is appropriate for simulating contaminant migration in soil and can be used to model vadose zone attenuation of leachate concentrations derived from a partition equation (see Section 2.5.1). In addition, since it links the output from the unsaturated zone transport module with a saturated zone module, it can be used to determine the concentration of a contaminant in a well located downgradient from a contaminant source. MULTIMED is appropriate for early-stage site simulations because the input parameters required are typically available and uncertainty analyses can be performed using Monte Carlo simulations for those parameters for which reliable values are not known.

VLEACH. In VLEACH, biological or chemical degradation is not considered. It therefore provides conservative estimates of contaminant migration in soil. This model may be appropriate as an initial screening tool for sites for which there is little information available. VLEACH can estimate volatile emissions (see Section 3.1) and can consider a finite source. It is therefore potentially applicable to both subsurface pathways addressed by the soil screening process.

SESOIL. SESOIL was designed as a screening tool, but it is actually more complex than some of the models described. Some of the input data would be cumbersome to obtain, especially for use as an initial screening tool. It is applicable for simulating spill sites since it allows consideration of surface transport by erosion and runoff and can utilize detailed meteorologic information to estimate infiltration. In the soil zone, several fate and transport options are available such as metal complexation, hydrolysis, cation exchange, and degradation. This model is especially applicable to sites where significant subsurface and meteorologic information is available. Although the model does consider volatilization from surface soils, the available documentation (Criscenti et al., 1994) is not clear as to whether it produces an output of volatile flux to the atmosphere.

PRZM-2. PRZM-2 is a relatively detailed model as a result of the coupling of the two models PRZM and VADOFT. Although PRZM is predominantly used as a pesticide leaching model, it could also be used for simulation of transport of other chemicals. Because detailed meteorology and surface application parameters can be included, it is appropriate for simulation of surface spills or land disposal scenarios. In addition, uncertainty analyses can be performed based on Monte Carlo simulations. Numerous subsurface fate and transport options exist in PRZM. Water movement is somewhat simplified in PRZM, and it may not be applicable for low-permeability soils (Criscenti et al., 1994). However, water flow simulation is more detailed in the VADOFT module of the PRZM-2 program. The combination of these programs makes PRZM-2 a relatively complex model. This model is especially applicable to sites for which significant site and meteorologic data are available.

Part 4: MEASURING CONTAMINANT CONCENTRATIONS IN SOIL

The Soil Screening Guidance includes a sampling strategy for implementing the soil screening process. Section 4.1 presents the sampling approach for surface soils. This approach provides a simple decision rule based on comparing the maximum contaminant concentrations of composite samples with surface soil screening levels (the Max test) to determine whether further investigation is needed for a particular exposure area (EA). In addition, this section presents a more complex strategy (the Chen test) that allows the user to design a site-specific quantitative sampling strategy by varying decision error limits and soil contaminant variability to optimize the number of samples and composites. Section 4.2 provides a subsurface soil sampling strategy for developing SSLs and applying the screening procedure for the volatilization and migration to ground water exposure pathways.

Section 4.3 describes the technical details behind the development of the SSL sampling strategy, including analyses and response to public and peer-review comments received on the December 1994 draft guidance.

The sampling strategy for the soil screening process is designed to achieve the following objectives:

- Estimate mean concentrations of contaminants of concern for comparison with SSLs

- Fill in the data gaps in the conceptual site model necessary to develop SSLs.

The soils of interest for the first objective differ according to the exposure pathway being addressed. For the direct ingestion, dermal, and fugitive dust pathways, EPA is concerned about surface soils. The sampling goal is to determine average contaminant concentrations of surface soils in exposure areas of concern. For inhalation of volatiles, migration to ground water and, in some cases, plant uptake, subsurface soils are the primary concern. For these pathways, the average contaminant concentration through each source is the parameter of interest.

The second objective (filling in the data gaps) applies primarily to the inhalation and migration to ground water pathways. For these pathways, the source area and depth as well as average soil properties within the source are needed to calculate the pathway-specific SSLs. Therefore, the sampling strategy needs to address collection of these site-specific data.

Because of the difference in objectives, the sampling strategies for the ingestion pathway and for the inhalation and migration to ground water pathways are addressed separately. If both surface and subsurface soils are a concern, then surface soils should be sampled first because the results of surface soil analyses may help delineate source areas to target for subsurface sampling.

At some sites, a third sampling objective may be appropriate. As discussed in the Soil Screening Guidance, SSLs may not be useful at sites where background contaminant levels are above the SSLs. Where sampling information suggests that background contaminant concentrations may be a concern, background sampling may be necessary. *Methods for Evaluating the Attainment of Cleanup Standards - Volume 3: Reference-Based Standards for Soil and Solid Media* (U.S. EPA, 1994e) provides further information on sampling soils to determine background conditions at a site.

In order to accurately represent contaminant distributions at a site, EPA used the Data Quality Objectives (DQO) process (Figure 4) to develop a sampling strategy that will satisfy Superfund program objectives. The DQO process is a systematic data collection planning process developed by EPA to ensure that the right type, quality, and quantity of data are collected to support EPA decision making. As shown in Sections 4.1.1 through 4.1.6, most of the key outputs of the DQO process already have been developed as part of the Soil Screening Guidance. The DQO activities addressed in this section are described in detail in the *Data Quality Objectives for Superfund: Interim Final Guidance* (U.S. EPA, 1993b) and the *Guidance for the Data Quality Objectives Process* (U.S. EPA, 1994c). Refer to these documents for more information on how to complete each DQO activity or how to develop other, site-specific sampling strategies.

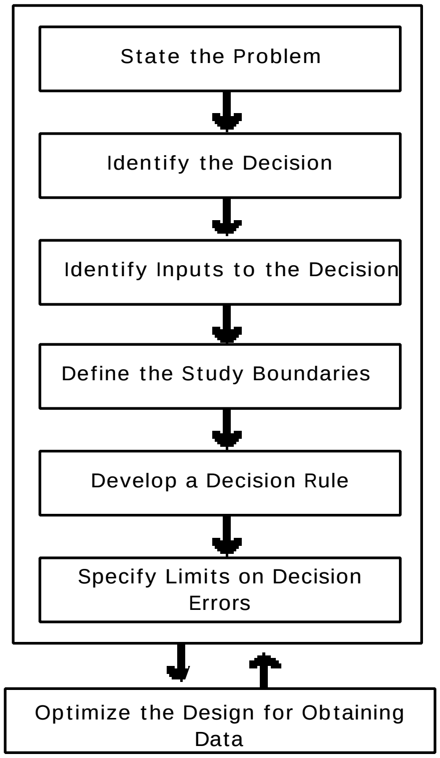


Figure 4. The Data Quality Objectives process.

4.1 Sampling Surface Soils

A sampling strategy for surface soils is presented in this section, organized by the steps of the DQO process. The first five steps of this process, from defining the problem through developing the basic decision rule, are summarized in Table 21, and are described in detail in the first five subsections. The details of the two remaining steps of the DQO process, specifying limits on decision errors and optimizing the design, have been developed separately for two alternative hypothesis testing procedures (the Max test and the Chen method) and are presented in four (4.1.6, 4.1.7, 4.1.9, and 4.1.10) subsections. In addition, a data quality assessment (DQA) follows the DQO process step for optimizing the design. The DQA ensures that site-specific error limits are achieved. Sections 4.1.8 and 4.1.11 describe the DQA for the Max and Chen tests, respectively. The technical details behind the development of the surface soil sampling design strategy are explained in Section 4.3.

4.1.1 State the Problem. In screening, the problem is to identify the contaminants and exposure areas (EAs) that do not pose significant risk to human health so that future investigations can be focused on the areas and contaminants of concern at a site.

The main site-specific activities involved in this first step of the DQO process include identifying the data collection planning team (including technical experts and key stakeholders) and specifying the available resources. The list of technical experts and stakeholders should contain all key personnel who are involved with applying the Soil Screening Guidance at the site. Other activities in this step include developing the conceptual site model (CSM), identifying exposure scenarios, and preparing a summary description of the surface soil contamination problem. The User's Guide (U.S. EPA, 1996) describes these activities in with more detail.

4.1.2 Identify the Decision. The decision is to determine whether the mean surface soil concentrations exceed surface soil screening levels for specific contaminants within EAs. If so, the EA must be investigated further. If not, no further action is necessary under CERCLA for the specific contaminants in the surface soils of those EAs.

Table 21. Sampling Soil Screening DQOs for Surface Soils

DQO Process Steps	Soil Screening Inputs/Outputs
State the Problem	
Identify scoping team	Site manager and technical experts (e.g., toxicologists, risk assessors, statisticians, soil scientists)
Develop conceptual site model (CSM)	CSM development (described in Step 1 of the User's Guide, U.S. EPA, 1996)
Define exposure scenarios	Direct ingestion and inhalation of fugitive particulates in a residential setting; dermal contact and plant uptake for certain contaminants
Specify available resources	Sampling and analysis budget, scheduling constraints, and available personnel
Write brief summary of contamination problem	Summary of the surface soil contamination problem to be investigated at the site
Identify the Decision	
Identify decision	Do mean soil concentrations for particular contaminants (e.g., contaminants of potential concern) exceed appropriate screening levels?
Identify alternative actions	Eliminate area from further study under CERCLA or Plan and conduct further investigation
Identify Inputs to the Decision	
Identify inputs	Ingestion and particulate inhalation SSLs for specified contaminants Measurements of surface soil contaminant concentration
Define basis for screening	Soil Screening Guidance
Identify analytical methods	Feasible analytical methods (both field and laboratory) consistent with program-level requirements
Define the Study Boundaries	
Define geographic areas of field investigation	The entire NPL site (which may include areas beyond facility boundaries), except for any areas with clear evidence that no contamination has occurred
Define population of interest	Surface soils (usually the top 2 centimeters, but may be deeper where activities could redistribute subsurface soils to the surface)
Divide site into strata	Strata may be defined so that contaminant concentrations are likely to be relatively homogeneous within each stratum based on the CSM and field measurements
Define scale of decision making	Exposure areas (EAs) no larger than 0.5 acre each (based on residential land use)
Define temporal boundaries of study	Temporal constraints on scheduling field visits
Identify practical constraints	Potential impediments to sample collection, such as access, health, and safety issues
Develop a Decision Rule	
Specify parameter of interest	"True mean" (μ) individual contaminant concentration in each EA. (since the determination of the "true mean" would require the collection and analysis of many samples, the "Max Test" uses another sample statistic, the maximum composite concentration).
Specify screening level	Screening levels calculated using available parameters and site data (or generic SSLs if site data are unavailable).
Specify "if..., then..." decision rule	If the "true mean" EA concentration exceeds the screening level, then investigate the EA further. If the "true mean" is less than the screening level, then no further investigation of the EA is required under CERCLA.

4.1.3 Identify Inputs to the Decision. This step of the DQO process requires identifying the inputs to the decision process, including the basis for further investigation and the applicable analytical methods. The inputs for deciding whether to investigate further are the ingestion, dermal, and fugitive dust inhalation SSLs calculated for the site contaminants as described in Part 2 of this document, and the surface soil concentration measurements for those same contaminants. Therefore, the remaining task is to identify Contract Laboratory Program (CLP) methods and/or field methods for which the quantitation limits (QLs) are less than the SSLs. EPA recommends the use of field methods, such as soil gas surveys, immunoassays, or X-ray fluorescence, where applicable and appropriate as long as quantitation limits are below the SSLs. At least 10 percent of field samples should be split and sent to a CLP laboratory for confirmatory analysis (U.S. EPA, 1993d).

4.1.4 Define the Study Boundaries. This step of the DQO process defines the sample population of interest, subdivides the site into appropriate exposure areas, and specifies temporal or practical constraints on the data collection. The description of the population of interest must include the surface soil depth.

Sampling Depth. When measuring soil contamination levels at the surface for the ingestion and inhalation pathways, the top 2 centimeters is usually considered surface soil, as defined by *Urban Soil Lead Abatement Project* (U.S. EPA 1993f). However, additional sampling beyond this depth may be appropriate for surface soils under a future residential use scenario in areas where major soil disturbances can reasonably be expected as a result of landscaping, gardening, or construction activities. In this situation, contaminants that were at depth can be moved to the surface. Thus, it is important to be cognizant of local residential construction practices when determining the depth of surface soil sampling and to weigh the likelihood of that area being developed.

Subdividing the Site. This step involves dividing the site into areas or strata depending on the likelihood of contamination and identifying areas with similar contaminant patterns. These divisions can be based on process knowledge, operational units, historical records, and/or prior sampling. Partitioning the site into such areas and strata can lead to a more efficient sampling design for the entire site.

For example, the site manager may have documentation that large areas of the site are unlikely to have been used for waste disposal activities. These areas would be expected to exhibit relatively low variability and the sampling design could involve a relatively small number of samples. The greatest intensity of sampling effort would be expected to focus on areas of the site where there is greater uncertainty or greater variability associated with contamination patterns. When relatively large variability in contaminant concentrations is expected, more samples are required to determine with confidence whether the EA should be screened out or investigated further.

Initially, the site may be partitioned into three types of areas:

1. Areas that are not likely to be contaminated
2. Areas that are known to be highly contaminated
3. Areas that are suspected to be contaminated and cannot be ruled out.

Areas that are not likely to be contaminated generally will not require further investigation if this assumption is based on historical site use information or other site data that are reasonably complete and accurate. (However, the site manager may also want take a few samples to confirm this assumption). These may be parts of the site that are within the legal boundaries of the property but were completely undisturbed by hazardous-waste-generating activities. All other areas need investigation.

Areas that are known to be highly contaminated (i.e., sources) are targeted for subsurface sampling. The information collected on source area and depth is used to calculate site-specific SSLs for the inhalation and migration to ground water pathways (see Section 4.2 for more information).

Areas that are suspected to be contaminated (and cannot be ruled out for screening) are the primary subjects of the surface soil investigation. If a geostatistician is available, a geostatistical model may be used to characterize these areas (e.g., kriging model). However, guidance for this type of design is beyond the scope of the current guidance (see Chapter 10 of U.S. EPA, 1989a).

Defining Exposure Areas. After the site has been partitioned into relatively homogeneous areas, each region that is targeted for surface soil sampling is then subdivided into EAs. An EA is defined as that geographical area in which an individual may be exposed to contamination over time. Because the SSLs were developed for a residential scenario, EPA assumes the EA is a suburban residential lot corresponding to 0.5 acre. For soil screening purposes, each EA should be 0.5 acre or less. To the extent possible, EAs should be constructed as square or rectangular areas that can be subdivided into squares to facilitate compositing and grid sampling. If the site is currently residential, then the EA should be the actual residential lot size. The exposure areas should not be laid out in such a way that they unnecessarily combine areas of high and low levels of contamination. The orientation and exact location of the EA, relative to the distribution of the contaminant in the soil, can lead to instances where sampling of the EA may lead to results above the mean, and other instances, to results below the mean. Try to avoid straddling contaminant “distribution units” within the 0.5 acre EA.

The sampling strategy for surface soils allows investigators to determine mean soil contaminant concentration across an EA of interest. An arithmetic mean concentration for an EA best represents the exposure to site contaminants over a long period of time. For risk assessment purposes, an individual is assumed to move randomly across an EA over time, spending equivalent amounts of time in each location. Since reliable information about specific patterns of nonrandom activity for future use scenarios is not available, random exposure appears to be the most reasonable assumption for a residential exposure scenario. Therefore, spatially averaged surface soil concentrations are used to estimate mean exposure concentrations.

Because all the EAs within a given stratum should exhibit similar contaminant concentrations, one site-specific sampling design can be developed for all EAs within that stratum. As discussed above, some strata may have relatively low variability and other strata may have relatively high variability. Consequently, a different sampling design may be necessary for each stratum, based upon the stratum-specific estimate of the contaminant variability.

4.1.5 Develop a Decision Rule. Ideally, the decision rule for surface soils is:

> If the mean contaminant concentration within an EA exceeds the screening level,
> then investigate that EA further.

This "screening level" is the actual numerical value used to compare against the site contamination data. It may be identical to the SSL, or it may be a multiple of the SSL (e.g., 2 SSL) for a hypothesis test designed to achieve specified decision error rates in a specified region above and below the SSL. In addition, another sample statistic (e.g., the maximum concentration) may be used as an estimate of the mean for comparison with the "screening level."

4.1.6 Specify Limits on Decision Errors for the Max Test. Sampling data will be used to support a decision about whether an EA requires further investigation. Because of variability in contaminant concentrations within an EA, practical constraints on sample sizes, and sampling or measurement error, the data collected may be inaccurate or nonrepresentative and may mislead the decision maker into making an incorrect decision. A decision error occurs when sampling data mislead the decision maker into choosing a course of action that is different from or less desirable than the course of action that would have been chosen with perfect information (i.e., with no constraints on sample size and no measurement error).

EPA recognizes that data obtained from sampling and analysis are never perfectly representative and accurate, and that the costs of trying to achieve near-perfect results can outweigh the benefits. Consequently, EPA acknowledges that uncertainty in data must be tolerated to some degree. The DQO process controls the degree to which uncertainty in data affects the outcomes of decisions that are based on those data. This step of the DQO process allows the decision maker to set limits on the probabilities of making an incorrect decision.

The DQO process utilizes hypothesis tests to control decision errors. When performing a hypothesis test, a presumed or baseline condition, referred to as the "null hypothesis" (H_o), is established. This baseline condition is presumed to be true unless the data conclusively demonstrate otherwise, which is called "rejecting the null hypothesis" in favor of an alternative hypothesis. For the Soil Screening Guidance, the baseline condition, or H_o, is that **the site needs further investigation.**

When the hypothesis test is performed, two possible decision errors may occur:

1. Decide not to investigate an EA further (i.e., "walk away") when the correct decision (with complete and perfect information) would be to "investigate further"

2. Decide to investigate further when the correct decision would be to "walk away."

Since the site is on the NPL, site areas are presumed to need further investigation. Therefore, the data must provide clear evidence that it would be acceptable to "walk away." This presumption provides the basis for classifying the two types of decision errors. The "incorrectly walk away" decision error is designated as the Type I decision error because one has incorrectly rejected the baseline condition (null hypothesis). Correspondingly, the "unnecessarily investigate further" decision error is designated as the Type II decision error.

To complete the specification of limits on decision errors, Type I and Type II decision error probability limits must be defined in relation to the SSL. First a "gray region" is specified with respect to the mean contaminant concentration within an EA. The gray region represents the range of contaminant levels near the SSL, where uncertainty in the data (i.e., the variability) can make the decision "too close to call." In other words, when the average of the data values is very close to the SSL, it would be too expensive to generate a data set of sufficient size and precision to resolve what the correct determination should be. (i.e., Does the average concentration fall "above" or "below" the SSL?)

The Soil Screening Guidance establishes a default range for the width and location of the "gray region": from one-half the SSL (0.5 SSL) to two times the SSL (2 SSL). By specifying the upper edge of the gray region as twice the SSL, it is possible that exposure areas with mean values slightly higher than the SSL may be screened from further study. However, EPA believes that the exposure scenario and assumptions used to derive SSLs are sufficiently conservative to be protective in such cases.

On the lower side of the gray region, the consequences of decision errors at one-half the SSL are primarily financial. If the lower edge of the gray region were to be moved closer to the SSL, then more exposure areas that were truly below the SSL would be screened out, but more money would be spent on sampling to make this determination. If the lower edge of the gray region were to be moved closer to zero, then less money could be spent on sampling, but fewer EAs that were truly below the SSLs would be screened out, leading to unnecessary investigation of EAs. The Superfund program chose the gray region to be one-half to two times the SSL after investigating several different ranges. This range for the gray region represents a balance between the costs of collecting and analyzing soil samples and making incorrect decisions. While it is desirable to estimate exactly the exposure area mean, the number of samples required are much more than project managers are generally willing to collect in a "screening" effort. Although some exposure areas will have contaminant concentrations that are between the SSL and twice the SSL and will be screened out, human health will still be protected given the conservative assumptions used to derive the SSLs.

The Soil Screening Guidance establishes the following goals for Type I and Type II decision error rates:

- Prob ("walk away" when the true EA mean is 2 SSL) = 0.05
- Prob ("investigate further" when the true EA mean is 0.5 SSL) = 0.20.

This means that there should be no more than a 5 percent chance that the site manager will "walk away" from an EA where the true mean concentration is 2 SSL or more. In addition, there should be no more than a 20 percent chance that the site manager will unnecessarily investigate an EA when the mean is 0.5 SSL or less.

These decision error limits are general goals for the soil screening process. Consistent with the DQO process, these goals may be adjusted on a site-specific basis by considering the available resources (i.e., time and budget), the importance of screening surface soil relative to other potential exposure pathways, consequences of potential decision errors, and consistency with other relevant EPA guidance and programs.

Table 22 summarizes this step of the DQO process for the Max test, specifying limits on the decision error rates, and the final step of the DQO process for the Max test, optimizing the design. Figure 5 illustrates the gray region for the decision error goals: a Type I decision error rate of 0.05 (5 percent) at 2 SSL and a Type II decision error rate of 0.20 (20 percent) at 0.5 SSL.

4.1.7 Optimize the Design for the Max Test. This section provides instructions for developing an optimum sampling strategy for screening surface soils. It discusses compositing, the selection of sampling points for composited and uncomposited surface soil sampling, and the recommended procedures for determining the sample sizes necessary to achieve specified limits on decision errors using the Max test.

Table 22. Sampling Soil Screening DQOs for Surface Soils under the Max Test

DQO Process Steps	Soil Screening Inputs/Outputs
Specify Limits on Decision Errors*	
Define baseline condition (null hypothesis)	The EA needs further investigation
Define the gray region**	From 0.5 SSL to 2 SSL
Define Type I and Type II decision errors	Type I error: Do not investigate further ("walk away from") an EA whose true mean exceeds the screening level of 2 SSL Type II error: Investigate further when an EA's true mean falls below the screening level of 0.5 SSL
Identify consequences	Type I error: potential public health consequences Type II error: unnecessary expenditure of resources to investigate further
Assign acceptable probabilities of Type I and Type II decision errors	Goals: Type I: 0.05 (5%) probability of not investigating further when “true mean” of the EA is 2 SSL Type II: 0.20 (20%) probability of investigating further when “true mean” of the EA is 0.5 SSL
Define QA/QC goals	CLP precision and bias requirements 10% CLP analyses for field methods
Optimize the Design	
Determine how to best estimate “true mean”	Samples composited across the EA estimate the EA mean ($\bar{x}$). Use maximum composite concentration as a conservative estimate of the true EA mean.
Determine expected variability of EA surface soil contaminant concentrations	A conservatively large expected coefficient of variation (CV) from prior data for the site, field measurements, or data from other comparable sites and expert judgment. A minimum default CV of 2.5 should be used when information is insufficient to estimate the CV.
Design sampling strategy by evaluating costs and performance of alternatives	Lowest cost sampling design option (i.e., compositing scheme and number of composites) that will achieve acceptable decision error rates
Develop planning documents for the field investigation	Sampling and Analysis Plan (SAP) Quality Assurance Project Plan (QAPjP)

* Since the DQO process controls the degree to which uncertainty in data affects the outcome of decisions that are based on that data, specifying limits on decision errors will allow the decision maker to control the probability of making an incorrect decision when using the DQOs.

** The gray region represents the area where the consequences of decision errors are minor (and uncertainty in sampling data makes decisions too close to call).

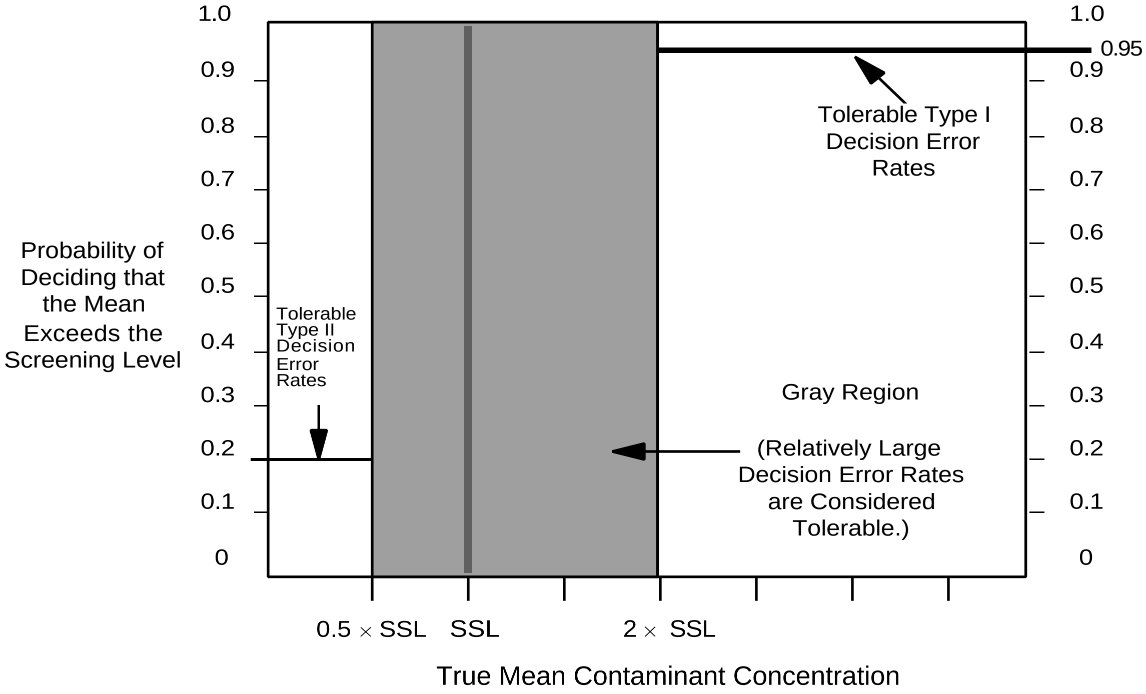


Figure 5. Design performance goal diagram.

Note that the size, shape, and orientation of sampling volume (i.e., "support") for heterogenous media have a significant effect on reported measurement values. For instance, particle size has a varying affect on the transport and fate of contaminants in the environment and on the potential receptors. Because comparison of data from methods that are based on different supports can be difficult, defining the sampling support is important in the early stages of site characterization. This may be accomplished through the DQO process with existing knowledge of the site, contamination, and identification of the exposure pathways that need to be characterized. Refer to *Preparation of Soil Sampling Protocols: Sampling Techniques and Strategies* (U.S. EPA, 1992f) for more information about soil sampling support.

The SAP developed for surface soils should specify sampling and analytical procedures as well as the development of QA/QC procedures. To identify the appropriate analytical procedures, the screening levels must be known. If data are not available to calculate site-specific SSLs, then the generic SSLs in Appendix A should be used.

Compositing. Because the objective of surface soil screening is to ensure that the mean contaminant concentration does not exceed the screening level, the physical "averaging" that occurs during compositing is consistent with the intended use of the data. Compositing allows a larger number of locations to be sampled while controlling analytical costs because several discrete samples are physically mixed (homogenized) and one or more subsamples are drawn from the mixture and submitted for analysis. If the individual samples in each composite are taken across the EA, each composite represents an estimate of the EA mean.

A practical constraint to compositing in some situations is the heterogeneity of the soil matrix. The efficiency and effectiveness of the mixing process may be hindered when soil particle sizes vary widely or when the soil matrix contains foreign objects, organic matter, viscous fluids, or sticky material. Soil samples should not be composited if matrix interference among contaminants is likely (e.g., when the presence of one contaminant biases analytical results for another).

Before individual specimens are composited for chemical analysis, the site manager should consider homogenizing and splitting each specimen. By compositing one portion of each specimen with the other specimens and storing one portion for potential future analysis, the spatial integrity of each specimen is maintained. If the concentration of a contaminant in a composite sample is high, the splits of the individual specimens from which it was composed can be analyzed discretely to determine which individual specimen(s) have high concentrations of the contaminant. This will permit the site manager to determine which portion within an EA is contaminated without making a repeat visit to the site.

Sample Pattern. The Max test should only be applied using composite samples that are representative of the entire EA. However, the Chen test (see Section 4.1.9) can be applied with individual, uncomposited samples. There are several options for developing a sampling pattern for compositing that produce samples that should be representative. If individual, uncomposited samples will be analyzed for contaminant concentrations, the N sample points can be selected using either (1) simple random sampling (SRS), (2) stratified SRS, or (3) systematic grid sampling (square or rectangular grid) with a random starting point (SyGS/rs). Step-by-step procedures for selecting SRS and SyGS/rs samples are provided in Chapter 5 of the U.S. EPA (1989a) and Chapter 5 of U.S. EPA (1994e). If stratified random sampling is used, the sampling rate must be the same in every sector, or stratum of the EA. Hence, the number of sampling points assigned to a stratum must be directly proportional to the surface area of the stratum.

Systematic grid sampling with a random starting point is generally preferred because it ensures that the sample points will be dispersed across the entire EA. However, if the boundaries of the EA are irregular (e.g., around the perimeter of the site or the boundaries of a stratum within which the EAs were defined), the number of grid sample points that fall within the EA depends on the random starting point selected. Therefore, for these irregularly shaped EAs, SRS or stratified SRS is recommended. Moreover, if a systematic trend of contamination is suspected across the EA (e.g., a strip of higher contamination), then SRS or stratified SRS is recommended again. In this case, grid sampling would be likely to result in either over- or under representation of the strip of higher contaminant levels, depending on the random starting point.

For composite sampling, the sampling pattern used to locate the discrete sample specimens that form each composite sample (N) is important. The composite samples should be formed in a manner that is consistent with the assumptions underlying the sample size calculations. In particular, each composite sample should provide an unbiased estimate of the mean contaminant concentration over the entire EA. One way to construct a valid composite of C specimens is to divide the EA into C sectors, or strata, of equal area and select one point at random from each sector. If sectors (strata) are of unequal sizes, the simple average is no longer representative of the EA as a whole.

Five valid sampling patterns and compositing schemes for selecting N composite samples that each consist of C specimens are listed below:

1. Select an SRS consisting of C points and composite all specimens associated with these points into a sample. Repeat this process N times, discarding any points that were used in a previous sample.

2. Select an SyGS/rs of C points and composite all specimens associated with the points in this sample. Repeat this process N times, using a new randomly selected starting point each time.

3. Select a single SyGS/rs of C×N points and use the systematic compositing scheme that is described in Highlight 3 to form N composites, as illustrated in Figure 6.

4. Select a single SyGS/rs of C×N points and use the random compositing scheme that is described in Highlight 4 to form N composites, as illustrated in Figure 7.

5. Select a stratified random sample of C×N points and use a random compositing scheme, as described in Highlight 5, to form N composites, as illustrated in Figure 8.

Methods 1, 2, and 5 are the most statistically defensible, with method 5 used as the default method in the Soil Screening Guidance. However, given the practical limits of implementing these methods, either method 3 or 4 is generally recommended for EAs with regular boundaries (e.g., square or rectangular). As noted above, if the boundaries of the EA are irregular, SyGS/rs sampling may not result in exactly C×N sample points. Therefore, for EAs with irregular boundaries, method 5 is recommended. Alternatively, a combination of methods 4 and 5 can be used for EAs that can be partitioned into C sectors of equal area of which K have regular boundaries and the remaining C - K have irregular boundaries.

Additionally, compositing within sectors to indicate whether one sector of the EA exceeds SSLs is an option that may also be considered. See Section 4.3.6 for a full discussion.

Sample Size. This section presents procedures to determine sample size requirements for the Max test that achieve the site-specific decision error limits discussed in Section 4.1.6. The Max test is based on the maximum concentration observed in N composite samples that each consist of C individual specimens. The individual specimens are selected so that each of the N composite samples is representative of the site as a whole, as discussed above. Hence, this section addresses determining the sample size pair, C and N, that achieves the site-specific decision error limits. Directions for performing the Max test in a manner that is consistent with DQOs established for a site are presented later in this section.

Table 23 presents the probabilities of Type I errors at 2 SSL and Type II errors at 0.5 SSL (the boundary points of the gray region discussed in Section 4.1.6) for several sample size options when the variability for concentrations of individual measurements across the EA ranges from 100 percent to 400 percent (CV = 1.0 to 4.0). Two choices for the number, C, of specimens per composite are shown in this table: 4 and 6. Fewer than four specimens per composite is not considered sufficient for the Max test. Fewer than four specimens per composite does not achieve the decision error limit goals for the level of variability generally encountered at CERCLA sites. More than six specimens may be more than can be effectively homogenized into a composite sample.

The number, N, of composite samples shown in Table 23 ranges from 4 to 9. Fewer than four samples is not considered sufficient because, considering decision error rates from simulation results (Section 4.3), the Max text should be based on at least four independent estimates of the EA mean. More than nine composite samples per EA is generally unlikely for screening surface soils at Superfund sites. However, additional sample size options can be determined from the simulation results reported in Appendix I.

Highlight 3: Procedure for Compositing of Specimens from a Grid Sample Using a Systematic Scheme (Figure 6)

1. Lay out a square or triangular grid sample over the EA, using a random start. Step-by-step procedures can be found in Chapter 5 of U.S. EPA (1989a). The number of points in the grid should be equal to C×N, where C is the desired number of specimens per composite and N is the desired number of composites.

2. Divide the EA into C sectors (strata) of equal area and shape such that each sector contains the same number of sample points. The number of sectors (C) should be equal to the number of specimens in each composite (since one specimen per area will be used in each composite) and the number of points within each sector, N, should equal the desired number of composite samples.

3. Label the points within one sector in any arbitrary fashion from 1 to N. Use the same scheme for each of the other sectors.

4. Form composite number 1 by compositing specimens with the '1' label, form composite number 2 by compositing specimens with the '2' label, etc. This leads to N composite samples that are subjected to chemical analysis.

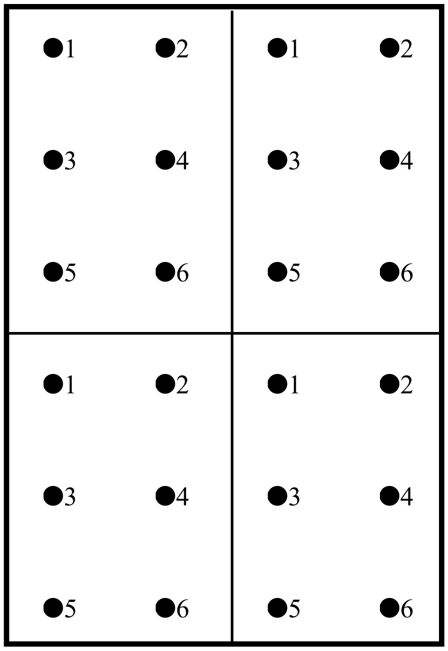


Figure 6. Systematic (square grid points) sample with systematic compositing scheme (6 composite samples consisting of 4 specimens).

Highlight 4: Procedure for Compositing of Specimens from a Grid Sample Using a Random Scheme (Figure 7)

1. Lay out a square or triangular grid sample over the EA, using a random start. Step-by-step procedures can be found in Chapter 5 of U.S. EPA (1989a). The number of points in the grid should be equal to C×N, where C is the desired number of specimens per composite and N is the desired number of composites.

2. Divide the EA into C sectors (strata) of equal area and shape such that each sector contains the same number of sample points. The number of sectors (C) should be equal to the number of specimens in each composite (since one specimen per area will be used in each composite) and the number of points within each sector, N, should equal the desired number of composite samples.

3. Use a random number table or random number generator to establish a set of labels for the N points within each sector. This is done by first labeling the points in a sector in an arbitrary fashion (say, points A, B, C,...) and associating the first random number with point A, the second with point B, etc. Then rank the points in the sector according to the set of random numbers and relabel each point with its rank. Repeat this process for each sector.

4. Form composite number 1 by compositing specimens with the ‘1’ label, form composite number 2 by compositing specimens with the ‘2’ label, etc. This leads to N composite samples that are subjected to chemical analysis.

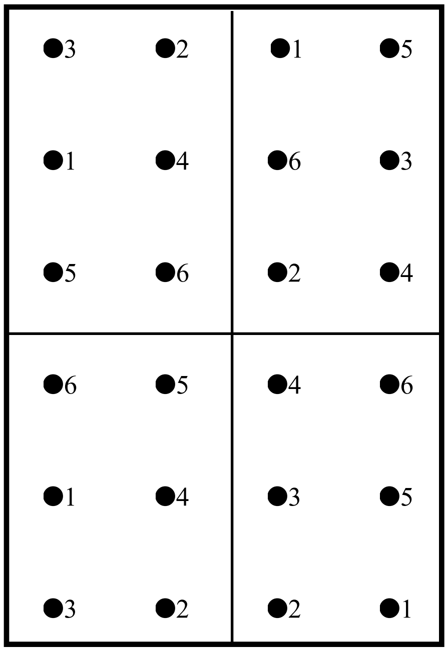


Figure 7. Systematic (square grid points) sample with random compositing scheme (6 composite samples consisting of 4 specimens).

Highlight 5: Procedure for Compositing of Specimens from a Stratified Random Sample Using a Random Scheme (Figure 8)

1. Divide the EA into C sectors (strata) of equal area, where C is equal to the number of specimens to be in each composite (since one specimen per stratum will be used in each composite).

2. Within each stratum, choose N random locations, where N is the desired number of composites. Step-by-step procedures for choosing random locations can be found in Chapter 5 of U.S. EPA (1989a).

3. Use a random number table or random number generator to establish a set of labels for the N points within each sector. This is done by first labeling the points in a sector in an arbitrary fashion (say, points A, B, C,...) and associating the first random number with point A, the second with point B, etc. Then rank the points in the sector according to the set of random numbers and relabel each point with its rank. Repeat this process for each sector.

4. Form composite number 1 by compositing specimens with the '1' label, form composite number 2 by compositing specimens with the '2' label, etc. This leads to N composite samples that are subjected to chemical analysis.

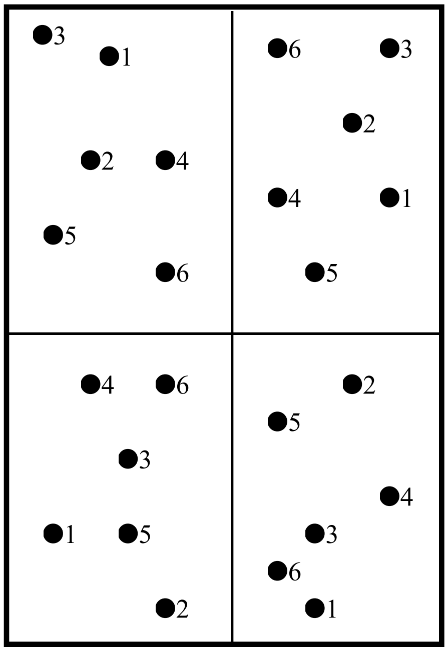


Figure 8. Stratified random sample with random compositing scheme (6 composite samples consisting of 4 specimens).

Table 23. Probability of Decision Error at 0.5 SSL and 2 SSL Using Max Test

	CV=1.0[a]		CV=1.5		CV=2.0		CV=2.5		CV=3.0		CV=3.5		CV=4.0	
Sample Size[b]	$E_{0.5}$[c]	$E_{2.0}$[d]	$E_{0.5}$	$E_{2.0}$	$E_{0.5}$	$E_{2.0}$	$E_{0.5}$	$E_{2.0}$	$E_{0.5}$	$E_{2.0}$	$E_{0.5}$	$E_{2.0}$	$E_{0.5}$	$E_{2.0}$
	C = 4 specimens per composite[e]													
4	<.01	0.08	0.02	0.11	0.09	0.13	0.14	0.19	0.19	0.20	0.24	0.26	0.25	0.30
5	<.01	0.05	0.02	0.06	0.11	0.10	0.15	0.10	0.26	0.17	0.26	0.18	0.31	0.25
6	<.01	0.03	0.02	0.04	0.11	0.06	0.21	0.08	0.28	0.11	0.31	0.11	0.35	0.16
7	<.01	0.01	0.03	0.02	0.12	0.04	0.25	0.05	0.31	0.08	0.36	0.09	0.41	0.15
8	<.01	0.01	0.03	0.01	0.16	0.02	0.25	0.04	0.36	0.05	0.42	0.07	0.41	0.09
9	<.01	0.01	0.05	0.01	0.16	0.01	0.28	0.03	0.36	0.04	0.44	0.07	0.48	0.08
	C = 6 specimens per composite													
4	<.01	0.08	<.01	0.11	0.03	0.12	0.08	0.16	0.15	0.17	0.26	0.20	0.23	0.27
5	<.01	0.05	<.01	0.06	0.04	0.09	0.11	0.09	0.17	0.13	0.22	0.15	0.25	0.20
6	<.01	0.03	0.01	0.04	0.06	0.04	0.14	0.06	0.19	0.09	0.25	0.09	0.29	0.12
7	<.01	0.01	0.01	0.02	0.06	0.02	0.14	0.04	0.23	0.06	0.29	0.08	0.37	0.08
8	<.01	0.01	0.01	0.01	0.06	0.02	0.15	0.02	0.25	0.03	0.30	0.04	0.40	0.06
9	<.01	0.01	0.01	0.01	0.06	0.01	0.18	0.02	0.28	0.03	0.34	0.03	0.39	0.04

[a] The CV is the coefficient of variation for individual, uncomposited measurements across the entire EA, including measurement error.

[b] Sample size (N) = number of composite samples.

[c] $E_{0.5}$ = Probability of requiring further investigation when the EA mean is 0.5 SSL.

[d] $E_{2.0}$ = Probability of not requiring further investigation when the EA mean is 2.0 SSL.

[e] C = number of specimens per composite sample, where each composite consists of points from a stratified random or systematic grid sample from across the entire EA.

NOTE: All decision error rates are based on 1,000 simulations that assume that each composite is representative of the entire EA, that half the EA has concentrations below the quantitation limit (i.e., SSL/100), and half the EA has concentrations that follow a gamma distribution (a conservative distributional assumption).

The error rates shown in Table 23 are based on the simulations presented in Appendix I. These simulations are based on the following assumptions:

1. Each of the N composite samples is based on C specimens selected to be representative of the EA as a whole, as specified above (C = number of sectors or strata).

2. One-half the EA has concentrations below the quantitation limit (which is assumed to be SSL/100).

3. One-half the EA has concentrations that follow a gamma distribution (see Section 4.3 for additional discussion).

4. Each chemical analysis is subject to a 20 percent measurement error.

The error rates presented in Table 23 are based on the above assumptions which make them robust for most potential distributions of soil contaminant concentrations. Distribution assumptions 2 and 3 were used because they were found in the simulations to produce high error rates relative to other potential contaminant distributions (see Section 4.3). If the proportion of the site below the quantitation limit (QL) is less than half or if the distribution of the concentration measurements is some other distribution skewed to the right (e.g., lognormal), rather than gamma, then the error rates achieved are likely to be no worse than those cited in Table 23. Although the actual contaminant distribution may be different from those cited above as the basis for Table 23, only extensive investigations will usually generate sufficient data to determine the actual distribution for each EA.

Using Table 23 to determine the sample size pair (C and N) needed to achieve satisfactory error rates with the Max test requires an *a priori* estimate of the coefficient of variation for measurements of the contaminant of interest across the EA. The coefficient of variation (CV) is the ratio of the standard deviation of contaminant concentrations for individual, uncomposited specimens divided by the EA mean concentration. As discussed in Section 4.1.4, the EAs should be constructed within strata expected to have relatively homogeneous concentrations so that an estimate of the CV for a stratum may be applicable for all EAs in that stratum. The site manager should use a conservatively large estimate of the CV for determining sample size requirements because additional sampling will be needed if the data suggest that the true CV is greater than that used to determine the sample sizes.

Potential sources of information for estimating the EA or stratum means, variances, and CVs include the following (in descending order of desirability):

- Data from a pilot study conducted at the site
- Prior sampling data from the site
- Data from similar sites
- Professional judgment.

For more information on estimating variability, see Section 6.3.1 of U.S. EPA (1989a).

4.1.8 Using the DQA Process: Analyzing Max Test Data.

This section provides guidance for analyzing the data for the Max test.

The hypothesis test for the Max test is very simple to implement, which is one reason that the Max test is attractive as a surface soil screening test. If x_1, x_2, ..., x_N represent concentration measurements for N composite samples that each consist of C specimens selected so that each composite is representative of the EA as a whole (as described in Section 4.1.7), the Max test is implemented as follows:

> If Max $(x_1, x_2, ..., x_N) \geq 2$ SSL, then investigate the EA further;
> If Max $(x_1, x_2, ..., x_N) < 2$ SSL, and the data quality assessment (DQA) indicates that the sample size was adequate, then no further investigation is necessary.

In addition, the step-by-step procedures presented in Highlight 6 must be implemented to ensure that the site-specific error limits, as discussed in Section 4.1.6, are achieved.

If the EA mean is below 2 SSL, the DQA process may be used to determine if the sample size was sufficiently large to justify the decision to not investigate further. To use Table 23 to check whether the sample size is adequate, an estimate of the CV is needed for each EA. The first four steps of Highlight 6, the DQA process for the Max test, present a process for the computation of a sample CV for an EA based on the N composite samples that each consist of C specimens.

However, the sample CV can be quite large when all the measurements are very small (e.g., well below the SSL) because CV approaches infinity as the EA sample mean ($\bar{x}$) approaches zero. Thus, when the composite concentration values for an EA are all near zero, the sample CV may be questionable and therefore unreliable for determining if the original sample size was sufficient (i.e., it could lead to further sampling when the EA mean is well below 2 SSL). To protect against unnecessary additional sampling in such cases, compare all composites against the equation given in Step 5 of Highlight 6. If the maximum composite sample concentration is below the value given by the equation, then the sample size may be assumed to be adequate and no further DQA is necessary.

To develop Step 5, EPA decided that if there were no compositing (C=1) and all the observations (based on a sample size appropriate for a CV of 2.5) were less than the SSL, then one can reasonably assume that the EA mean was not greater than 2 SSL. Likewise, because the standard error for the mean of C specimens, as represented by the composite sample, is proportional to $1/\sqrt{C}$, the comparable condition for composite observations is that one can reasonably assume that the EA mean was not greater than 2 SSL when all composite observations were less than SSL/$\sqrt{C}$. If this is the case for an EA sample set, the sample size can be assumed to be adequate and no further DQA is needed. Otherwise (when at lease one composite observation is not this small), use Table 23 with the sample CV for the EA to determine whether a sufficient number of samples were taken to achieve DQOs.

In addition to being simple to implement, the Max test is recommended because it provides good control over the Type I error rates at 2 SSL with small sample sizes. It also does not need any assumptions regarding observations below the QL. Moreover, the Max test error rates at 2 SSL are fairly robust against alternative assumptions regarding the distribution of surface soil concentrations in the EA. The simulations in Appendix I show that these error rates are rather stable for lognormal or Weibull contaminant concentration distributions and for different assumptions about portions of the site with contaminant concentrations below the QL.

Highlight 6: Directions for Data Quality Assessment for the Max Test

Let $x_1, x_2, ..., x_N$ represent contaminant concentration measurements for N composite samples that each consist of C specimens selected so that each composite is representative of the EA as a whole. The following describes the steps required to ensure that the Max test achieves the DQOs established for the site.

STEP 1: The site manager determines the Type I error rate to be achieved at 2 SSL and the Type II error rate to be achieved at 0.5 SSL, as described in Section 4.1.6.

STEP 2: Calculate the sample mean $\bar{x} = \left[\sum_{i=1}^{N} x_i \right] \frac{1}{N}$

STEP 3: Calculate the sample standard deviation

$$s = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} \left(x_i - \bar{x} \right)^2}$$

STEP 4: Calculate the sample estimate of the coefficient of variation, CV, for individual concentration measurements from across the EA.

$$CV = \frac{\sqrt{C}\ s}{\bar{x}}$$

NOTE: This is a conservation approximation of the CV for individual measurements.

STEP 5: If Max $(x_1, x_2, ..., x_N) < \frac{SSL}{\sqrt{C}}$, then no further data quality assessment is needed and the EA needs no further investigation.

Otherwise proceed to Step 6.

STEP 6: Use the value of the sample CV calculated in Step 4 as the true CV of concentrations to determine which column of Table 23 is applicable for determining sample size requirements. Using the error limits established in Step 1, determine the sample size requirements from this table. If the required sample size is greater than that implemented, further investigation of the EA is necessary. The further investigation may consist of selecting a supplemental sample and repeating the Max test with the larger, combined sample.

A limitation of the Max test is that it does not provide as good control over the Type II error rates at 0.5 SSL as it does for Type I error rates at 2 SSL. In fact, for a fixed number, C, of specimens per composite, the Type II error rate increases as the number of composite samples, N, increases. As the sample size increases, the likelihood of observing an unusual sample with the maximum exceeding 2 SSL increases. However, the Type II error rate can be decreased by increasing the number of specimens per composite. This unusual performance of the Max test as a hypothesis testing procedure occurs because the rejection region is fixed below 2 SSL and thus does not depend on the sample size (as it does for typical hypothesis testing procedures).

4.1.9 Specify Limits on Decision Errors for Chen Test. Although the Max test is adequate and appropriate for selecting a sample size for site screening, there are other alternate methods of screening surface soils. One such alternate method is the Chen test. In general, the Chen test differs from the Max test in its basic assumption about site contamination and the purpose of soil sampling. Because of this variation, these two methods have different null hypotheses and different decision error types.

There are two formulations of the statistical hypothesis test concerning the true (but unknown) mean contaminant concentration, μ, that achieve the Soil Screening Guidance decision error rate goals specified in Section 4.1.6. They are:

1. Test the null hypothesis, H_0: $\mu \geq 2$ SSL, versus the alternative hypothesis, H_1: $\mu < 2$ SSL, at the 5 percent significance level using a sample size chosen to achieve a Type II error rate of 20 percent at 0.5 SSL.

2. Test the null hypothesis, H_0: $\mu \leq 0.5$ SSL, versus the alternative hypothesis, H_1: $\mu > 0.5$ SSL, at the 20 percent significance level using a sample size chosen to achieve a Type II error rate of 5 percent at 2 SSL.

The first formulation of the problem (which is commonly used in the Superfund program) has the advantage that the error rate that has potential public health consequences is controlled directly via the significance level of the test. The error rate that has primarily cost consequences can be reduced by increasing the sample size above the minimum requirement. However, EPA has identified a new test procedure, the Chen test (Chen, 1995), which requires the second formulation but is less sensitive to assumptions regarding the distribution of the contaminant measurements than the Land procedure used in the December 1994 draft Technical Background Document (see Section 4.3). This section provides guidance regarding application of the Chen test and is, therefore, based on the second formulation of the hypothesis test.

A disadvantage of the second formulation is its performance when the true EA mean is between 0.5 SSL and the SSL. In this case, as the sample size increases, the test indicates the decision to investigate further, even though the mean is less than the SSL. In fact, no test procedure with feasible sample sizes performs well when the true EA mean is in the "gray region" between 0.5 SSL and 2 SSL (see Section 4.3). Whenever large sample sizes are feasible, one should modify the problem statement and test the null hypothesis, H_0: $\mu \leq$ SSL, instead of H_0: $\mu \leq 0.5$ SSL. One would then develop appropriate DQOs for this modified hypothesis test (e.g., significance level of 20 percent at the SSL and 5 percent probability of decision error at 2 SSL).

When the true mean of an EA is compared with the screening level, there are two possible decision errors that may occur: (1) decide not to investigate an EA further (i.e., "walk away") when the correct decision would be to "investigate further"; and (2) decide to investigate further when the correct decision would be to "walk away." For the Chen test, the "incorrectly walk away" decision error is designated as the Type II decision error because it occurs when we incorrectly accept the null hypothesis. Correspondingly, the "unnecessarily investigate further" decision error is designated as the Type I decision error because it occurs when we incorrectly reject the null hypothesis.

As discussed in Section 4.1.6, the Soil Screening Guidance specifies a default gray region for decision errors from 0.5 SSL to 2 SSL and sets the following goals for Type I and Type II error rates:

- Prob ("investigate further" when the true EA mean is 0.5 SSL) = 0.20
- Prob ("walk away" when the true EA mean is 2 SSL) = 0.05.

Table 24 summarizes this step of the DQO process for the Chen test, specifying limits on the decision error rates, and the final step of the DQO process, optimizing the design.

4.1.10 Optimize the Design Using the Chen Test. This section includes guidance on developing an optimum sampling strategy for screening surface soils. It discusses compositing, the selection of sampling points for composited and uncomposited surface soil sampling, and the recommended procedures for determining the sample sizes necessary to achieve specified limits on decision errors using the Chen test.

Note that the size, shape, and orientation of sampling volume (i.e., “support”) for heterogenous media have a significant effect on reported measurement values. For instance, particle size has a varying affect on the transport and fate of contaminants in the environment and on the potential receptors. Because comparison of data from methods that are based on different supports can be difficult, defining the sampling support is important in the early stages of site characterization. This may be accomplished through the DQO process with existing knowledge of the site, contamination, and identification of the exposure pathways that need to be characterized. Refer to *Preparation of Soil Sampling Protocols: Sampling Techniques and Strategies* (U.S. EPA, 1992f) for more information about soil sampling support.

The SAP developed for surface soils should specify sampling and analytical procedures as well as the development of QA/QC procedures. To identify the appropriate analytical procedures, the screening levels must be known. If data are not available to calculate site-specific SSLs, then the generic SSLs in Appendix A should be used.

Compositing. Because the objective of surface soil screening is to ensure that the mean contaminant concentration does not exceed the screening level, the physical "averaging" that occurs during compositing is consistent with the intended use of the data. Compositing allows a larger number of locations to be sampled while controlling analytical costs because several discrete samples are physically mixed (homogenized) and one or more subsamples are drawn from the mixture and submitted for analysis. If the individual samples in each composite are taken across the EA, each composite represents an estimate of the EA mean.

A practical constraint to compositing in some situations is the heterogeneity of the soil matrix. The efficiency and effectiveness of the mixing process may be hindered when soil particle sizes vary widely or when the soil matrix contains foreign objects, organic matter, viscous fluids, or sticky material. Soil samples should not be composited if matrix interference among contaminants is likely (e.g., when the presence of one contaminant biases analytical results for another).

Table 24. Sampling Soil Screening DQOs for Surface Soils under Chen Test

DQO Process Steps	Soil Screening Inputs/Outputs
Specify Limits on Decision Errors	
Define baseline condition (null hypothesis)	EA needs no further investigation
Define gray region	From 0.5 SSL to 2 SSL
Define Type I and Type II decision errors	Type I error: Investigate further when an EA's true mean concentration is below 0.5 SSL Type II error: Do not investigate further ("walk away from") when an EA true mean concentration is above 2 SSL
Identify consequences	Type I error: unnecessary expenditure of resources to investigate further Type II error: potential public health consequences
Assign acceptable probabilities of Type I and Type II decision errors	Goals: Type I: 0.20 (20%) probability of investigating further when EA mean is 0.5 SSL Type II: 0.05 (5%) probability of not investigating further when EA mean is 2 SSL
Optimize the Design	
Determine expected variability of EA surface soil contaminant concentrations	A conservatively large expected coefficient of variation (CV) from prior data for the site, field measurements, or data from other comparable sites and expert judgment
Design sampling strategy by evaluating costs and performance of alternatives	Lowest cost sampling design option (i.e., compositing scheme and number of composites) that will achieve acceptable decision error rates
Develop planning documents for the field investigation	Sampling and Analysis Plan (SAP) Quality Assurance Project Plan (QAPjP)

Before individual specimens are composited for chemical analysis, the site manager should consider homogenizing and splitting each specimen. By compositing one portion of each specimen with the other specimens and storing one portion for potential future analysis, the spatial integrity of each specimen is maintained. If the concentration in a composite is high, the splits of the individual specimens of which it was composed can be analyzed subsequently to determine which individual specimen(s) have high concentrations. This will permit the site manager to determine which portion within an EA is contaminated without making a repeat visit to the site.

Sample Pattern. The Chen test can be applied using composite samples that are representative of the entire EA or with individual uncomposited samples.

Systematic grid sampling (SyGS) generally is preferred because it ensures that the sample points will be dispersed across the entire EA. However, if the boundaries of the EA are irregular (e.g., around the perimeter of the site or the boundaries of a stratum within which the EAs were defined), the number of grid sample points that fall within the EA depends on the random starting point selected. Therefore, for these irregularly shaped EAs, SRS or stratified SRS is recommended. Moreover, if a systematic trend of contamination is suspected across the EA (e.g., a strip of higher contamination), then SRS or stratified SRS is recommended again. In this case, grid sampling would be likely to result in either over- or under representation of the strip of higher contaminant levels, depending on the random starting point.

For composite sampling, the sampling pattern used to locate the C discrete sample specimens that form each composite sample is important. The composite samples must be formed in a manner that is consistent with the assumptions underlying the sample size calculations. In particular, each composite sample must provide an unbiased estimate of the mean contaminant concentration over the entire EA. One way to construct a valid composite of C specimens is to divide the EA into C sectors, or strata, of equal area and select one point at random from each sector. If sectors (strata) are of unequal sizes, the simple average is no longer representative of the EA as a whole.

Valid sampling patterns and compositing schemes for selecting N composite samples that each consist of C specimens include the following:

1. Select an SRS consisting of C points and composite all specimens associated with these points into a sample. Repeat this process N times, discarding any points that were used in a previous sample.

2. Select an SyGS/rs of C points and composite all specimens associated with the points in this sample. Repeat this process N times, using a new randomly selected starting point each time.

3. Select a single SyGS/rs of CN points and use the systematic compositing scheme that is described in Highlight 3 to form N composites, as illustrated in Figure 6.

4. Select a single SyGS/rs of C×N points and use the random compositing scheme that is described in Highlight 4 to form N composites, as illustrated in Figure 7.

5. Select a stratified random sample of C×N points and use a random compositing scheme, as described in Highlight 5, to form N composites, as illustrated in Figure 8.

Methods 1, 2, and 5 are the most statistically defensible, with method 5 used as the default method in the Soil Screening Guidance. However, given the practical limits of implementing these methods, either method 3 or 4 is generally recommended for EAs with regular boundaries (e.g., square or rectangular). As noted above, if the boundaries of the EA are irregular, SyGS/rs sampling may not result in exactly C×N sample points. Therefore, for EAs with irregular boundaries, method 5 is recommended. Alternatively, a combination of methods 4 and 5 can be used for EAs that can be partitioned into C sectors of equal area of which K have regular boundaries and the remaining C - K have irregular boundaries.

Sample Size. This section provides procedures to determine sample size requirements for the Chen test that achieve the site-specific decision error limits discussed in Section 4.1.6. The Chen test is an upper-tail test for the mean of positively skewed distributions, like the lognormal (Chen, 1995). It is based on the mean concentration observed in a simple random sample, or equivalent design, selected from a distribution with a long right-hand tail.

The Chen procedure is a hypothesis testing procedure that is robust among the family of right-skewed distributions (see Section 4.3). That is, decision error rates for a given sample size are relatively insensitive to the particular right-skewed distribution that generated the data. This robustness is important in the context of surface soil screening because the number of surface soil samples will usually not be sufficient to determine the distribution of the concentration measurements.

The procedures presented above for selecting composited or uncomposited simple random or systematic grid samples can all be used to generate samples for application of the Chen test. The Chen procedure is based on a simple random sample, or one that can be analyzed as if it were an SRS. Directions for performing the Chen test in a manner that is consistent with the DQOs that have been established for a site are presented later.

Tables 25 through 30 provide the sample sizes required for the Chen test performed at the 10, 20, or 40 percent levels of significance (probability of Type I error at 0.5 SSL) and achieve, at most, a 5 or 10 percent probability of (Type II) error at 2 SSL. The Type II error rates at 2 SSL are based on the simulations presented in Appendix I. These simulations are based on the following assumptions:

1. Each of the N composite samples is based on C specimens selected to be representative of the EA as a whole, as specified above.
2. One-half the EA has concentrations below the quantitation limit (which is assumed to be SSL/100).
3. One-half the EA has concentrations that follow a gamma distribution.
4. Measurements below the QL are replaced by 0.5 QL for computation of the Chen test statistic.
5. Each chemical analysis is subject to a 20 percent measurement error.

Distributional assumptions 2 and 3 were used as the basis for the Type II error rates at 2 SSL (shown in Tables 25 through 30) because they were found in the simulations to produce high error rates relative to other potential contaminant distributions. If the proportion of the site below the QL is less than half or if the distribution of the concentration measurements is some other right-skewed distribution (e.g., lognormal), rather than gamma, then the Type II error rates achieved are likely to be no worse than those cited in Tables 25 through 30. No sample sizes, N, less than four are shown in these tables (irrespective of the number of specimens per composite) because consideration of the simulation results presented in Section 4.3 has led to a program-level decision that at least four separate analyses are required to adequately characterize the mean of an EA. No sample sizes in excess of nine are presented because of a program-level decision that more than nine samples per exposure area is generally unlikely for screening surface soils at Superfund sites. However, additional sample size options can be determined from the simulations reported in Appendix I.

When using Tables 25 through 30 to determine the sample size pair (C and N) needed to achieve satisfactory error rates with the Chen test, investigators must have an *a priori* estimate of the CV for measurements of the contaminant of interest across the EA. As previously discussed for the Max test, the site manager should use a conservatively large estimate of the CV for determining sample size requirements because additional sampling will be required if the data suggest that the true CV is greater than that used to determine the sample sizes.

Table 25. Minimum Sample Size for Chen Test at 10 Percent Level of Significance to Achieve a 5 Percent Chance of "Walking Away" When EA Mean is 2.0 SSL, Given Expected CV for Concentrations Across the EA

Number of specimens per composite[b]	Coefficient of variation (CV)[a]				
	1.0	1.5	2.0	2.5	3.0
2	7	9	>9	>9	>9
3	5	7	9	>9	>9
4	4	6	8	>9	>9
5	4	5	6	8	>9
6	4	4	5	7	9

[a] The CV is the coefficient of variation for individual, uncomposited measurements across the entire EA and includes measurement error.

[b] Each composite consists of points from a stratified random or systematic grid sample across the entire EA.

NOTE: Sample sizes are based on 1,000 simulations that assume that each composite is representative of the entire EA, that half the EA has concentrations below the limit of detection, and that half the EA has concentrations following a gamma distribution (a conservative distributional assumption).

Table 26. Minimum Sample Size for Chen Test at 20 Percent Level of Significance to Achieve a 5 Percent Chance of "Walking Away" When EA Mean is 2.0 SSL, Given Expected CV for Concentrations Across the EA

Number of specimens per composite[b]	Coefficient of variation (CV)[a]					
	1.0	1.5	2.0	2.5	3.0	3.5
1	9	>9	>9	>9	>9	>9
2	5	7	>9	>9	>9	>9
3	4	5	7	9	>9	>9
4	4	4	6	7	>9	>9
5	4	4	4	6	8	>9
6	4	4	4	5	8	9

[a] The CV is the coefficient of variation for individual, uncomposited measurements across the entire EA and includes measurement error.

[b] Each composite consists of points from a stratified random or systematic grid sample across the entire EA.

NOTE: Sample sizes are based on 1,000 simulations that assume that each composite is representative of the entire EA, that half the EA has concentrations below the limit of detection, and that half the EA has concentrations following a gamma distribution (a conservative distributional assumption).

Table 27. Minimum Sample Size for Chen Test at 40 Percent Level of Significance to Achieve a 5 Percent Chance of "Walking Away" When EA Mean is 2.0 SSL, Given Expected CV for Concentrations Across the EA

Number of specimens per composite[b]	Coefficient of variation (CV)[a]						
	1.0	1.5	2.0	2.5	3.0	3.5	4.0
1	5	9	>9	>9	>9	>9	>9
2	4	4	8	9	>9	>9	>9
3	4	4	5	7	>9	>9	>9
4	4	4	4	5	8	>9	>9
5	4	4	4	5	6	9	>9
6	4	4	4	4	5	8	9

[a] The CV is the coefficient of variation for individual, uncomposited measurements across the entire EA and includes measurement error.

[b] Each composite consists of points from a stratified random or systematic grid sample across the entire EA.

NOTE: Sample sizes are based on 1,000 simulations that assume that each composite is representative of the entire EA, that half the EA has concentrations below the limit of detection, and that half the EA has concentrations following a gamma distribution (a conservative distributional assumption).

Table 28. Minimum Sample Size for Chen Test at 10 Percent Level of Significance to Achieve a 10 Percent Chance of "Walking Away" When EA Mean is 2.0 SSL, Given the Expected CV for Concentrations Across the EA

Number of specimens per composite[b]	Coefficient of variation (CV)[a]					
	1.0	1.5	2.0	2.5	3.0	3.5
2	6	7	>9	>9	>9	>9
3	4	5	7	>9	>9	>9
4	4	4	6	7	>9	>9
5	4	4	5	6	8	>9
6	4	4	4	5	7	9

[a] The CV is the coefficient of variation for individual, uncomposited measurements across the entire EA and includes measurement error.

[b] Each composite consists of points from a stratified random or systematic grid sample across the entire EA.

NOTE: Sample sizes are based on 1,000 simulations that assume that each composite is representative of the entire EA, that half the EA has concentrations below the limit of detection, and that half the EA has concentrations following a gamma distribution (a conservative distributional assumption).

Table 29. Minimum Sample Size for Chen Test at 20 Percent Level of Significance to Achieve a 10 Percent Chance of “Walking Away” When EA Mean is 2.0 SSL, Given Expected CV for Concentrations Across the EA

Number of specimens per composite[b]	Coefficient of variation (CV)[a]						
	1.0	1.5	2.0	2.5	3.0	3.5	4.0
1	7	9	>9	>9	>9	>9	>9
2	4	5	8	>9	>9	>9	>9
3	4	4	5	8	>9	>9	>9
4	4	4	4	5	8	>9	>9
5	4	4	4	5	6	8	>9
6	4	4	4	4	5	7	9

[a] The CV is the coefficient of variation for individual, uncomposited measurements across the entire EA and includes measurement error.

[b] Each composite consists of points from a stratified random or systematic grid sample across the entire EA.

NOTE: Sample sizes are based on 1,000 simulations that assume that each composite is representative of the entire EA, that half the EA has concentrations below the limit of detection, and that half the EA has concentrations following a gamma distribution (a conservative distributional assumption).

Table 30. Minimum Sample Size for Chen Test at 40 Percent Level of Significance to Achieve a 10 Percent Chance of “Walking Away” When EA Mean is 2.0 SSL, Given Expected CV for Concentrations Across the EA

Number of specimens per composite[b]	Coefficient of variation (CV)[a]						
	1.0	1.5	2.0	2.5	3.0	3.5	4.0
1	4	7	9	>9	>9	>9	>9
2	4	4	5	8	9	>9	>9
3	4	4	4	5	7	9	>9
4	4	4	4	4	5	7	>9
5	4	4	4	4	5	6	8
6	4	4	4	4	4	5	6

[a] The CV is the coefficient of variation for individual, uncomposited measurements across the entire EA and includes measurement error.

[b] Each composite consists of points from a stratified random or systematic grid sample across the entire EA.

NOTE: Sample sizes are based on 1,000 simulations that assume that each composite is representative of the entire EA, that half the EA has concentrations below the limit of detection, and that half the EA has concentrations following a gamma distribution (a conservative distributional assumption).

Given an *a priori* estimate of the CV of concentration measurements in the EA, the site manager can use Table 26 to determine a sample size option that achieves the decision error goals for surface soil screening presented in Section 4.1.6 (i.e., not more than 20 percent chance of error at 0.5 SSL and not more than 5 percent at 2 SSL). For example, suppose that the site manager expects that the maximum true CV for concentration measurements in an EA is 2. Then Table 26 shows that six composite samples, each consisting of four specimens, will be sufficient to achieve the decision error limit goals.

4.1.11 Using the DQA Process: Analyzing Chen Test Data. Step-by-step instructions for using the Chen test to analyze data from both discrete random samples and pseudo-random samples (e.g., composite samples constructed as described previously) are provided in Highlight 7. This method for analyzing the data is a robust procedure for an upper-tailed test for the mean of a positively skewed distribution. As explained by Chen (1995), this procedure is a robust generalization of the familiar Student's t-test; it further generalizes a method developed by Johnson (1978) for asymmetric distributions.

The only assumption necessary for valid application of the Chen procedure is that the sample be a random sample from a right-skewed distribution. This robustness within the broad family of right-skewed distributions is appropriate for screening surface soil because the distribution of concentrations within an EA may depart from the common assumption of lognormality.

Computation of the Chen test statistic, as shown in Highlight 7, requires that concentration values be available for all N individual or composite samples analyzed for the contaminant of interest. If an analytical test result is reported below the quantitation limit, it should be used in the computations. For results below detection, substitute one-half the QL.

A disadvantage of the Chen procedure is that the hypothesis, “the EA needs no further investigation,” must be treated as the alternative hypothesis, rather than as the null hypothesis. As a result, the Type I error rate at 0.5 SSL is controlled via the significance level of the test, rather than the error rate at 2 SSL, which may have public health consequences. Hence, if the sample sizes (C and N) are based on an assumed CV that is too small, the desired error rate at 2 SSL is likely not to be achieved. Therefore, it is important to perform the data quality assurance check specified in Steps 6 through 8 of Highlight 7 to ensure that the desired error rate at 2 SSL is achieved. Moreover, it is important that the site manager base the initial EA sample sizes on a conservatively large estimate of the CV so that this process will not result in the need for additional sampling.

4.1.12 Special Considerations for Multiple Contaminants. If the surface soil samples collected for an EA will be tested for multiple contaminants, be aware that the expected CVs for the different contaminants may not all be identical. A conservative approach is to base the sample sizes for all contaminants on the largest expected CV.

4.1.13 Quality Assurance/Quality Control Requirements. Regardless of the sampling approach used, the Superfund quality assurance program guidance must be followed to ensure that measurement error rates are documented and within acceptable limits (U.S. EPA, 1993d).

Highlight 7: Directions for the Chen Test Using Simple Random Sample Scheme

Let $x_1, x_2, \ldots, x_N$, represent concentration measurements for N random sampling points or N pseudo-random sampling points (i.e., from a design that can be analyzed as if it were a simple random sample). The following describes the steps for a one-sample test for H_o: $\mu \leq 0.5$ SSL at the $100\alpha\%$ significance level that is designed to achieve a $100\beta\%$ chance of incorrectly accepting H_o when $\mu = 2$ SSL.

STEP 1: Calculate the sample mean $\bar{x} = \left[\sum_{i=1}^{N} x_i \right] \frac{1}{N}$

STEP 2: Calculate the sample standard deviation

$$s = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} \left(x_i - \bar{x}\right)^2}$$

STEP 3: Calculate the sample skewness

$$b = N \frac{\sum_{i=1}^{N} \left(x_i - \bar{x} \right)^3}{(N-1)\ (N-2)\ s^3}$$

STEP 4: Calculate the Chen test statistic, t_2, as follows:

$$a = \frac{b}{6\sqrt{N}}$$

$$t = \frac{\bar{x} - 0.5\ \mathrm{SSL}}{s\ /\ \sqrt{N}}$$

$$t_2 = t + a\left(1 + 2t^2\right) + 4a^2\left(t + 2t^3\right)$$

STEP 5: Compare t_2 to z_α, the $100(1 - \alpha)$ percentile of the standard normal probability distribution.

If $t_2 > z_\alpha$, the null hypothesis is rejected, and the EA needs further investigation.

If $t_2 \leq z_\alpha$, there is insufficient evidence to reject the null hypothesis. Proceed to Step 6 to determine if the sample size is sufficient to achieve a $100\beta\%$ or less chance of incorrectly accepting the H_o when $\mu = 2$ SSL.

Highlight 7: Directions for the Chen Test Using Simple Random Sample Scheme (continued)

STEP 6: Let C represent the number of specimens composited to form each of the N samples, where each of $x_1, x_2, \ldots, x_N$ is a composite sample consisting of C specimens selected so that each composite is representative of the EA as a whole. (If each of $x_1, x_2, \ldots, x_N$ is an individual random or pseudo-random sampling point, then C = 1.)

If $\text{Max}\,(x_1, x_2, \ldots, x_N) < \frac{SSL}{\sqrt{C}}$, then no further data quality assessment is needed and the EA needs no further investigation.

Otherwise proceed to Step 7.

STEP 7: Calculate the sample estimate of the coefficient of variation, CV, for individual concentration measurements from across the EA.

$$CV = \frac{\sqrt{C}\ s}{\bar{x}}$$

NOTE: This calculation ignores measurement error, which results in conservatively large sample size requirements.

STEP 8: Use the value of the sample CV calculated in Step 7 as the true CV of concentrations in Tables 25 through 30 to determine the minimum sample size, N^*, necessary to achieve a 100ß% or less chance of incorrectly accepting H_0 when $\mu = 2$ SSL.

If $N \geq N^*$, the EA needs no further investigation.

If $N < N^*$, further investigation of the EA is necessary. The further investigation may consist of selecting a supplemental sample and repeating this hypothesis testing procedure with the larger, combined sample.

4.1.14 Final Analysis. After either the Max test or the Chen test has been performed for each EA of interest (0.5 acre or less) at an NPL site, the pattern of decisions for individual EAs (to "walk away" or to "investigate further") should be examined. If some EAs for which the decision was to "walk away" are surrounded by EAs for which the decision was to "investigate further," it may be more efficient to identify an area including all these EAs for further study and develop a global investigation strategy.

4.1.15 Reporting. The decision process for surface soil screening should be thoroughly documented as part of the RI/FS process. This documentation should include a map of the site (showing the boundaries of the EAs and the sectors, or strata, within EAs that were used to select sampling points within the EAs); documentation of how composite samples were formed and the number of composite samples that were analyzed for each EA; the raw analytical data; the results of all hypothesis tests; and the results of all QA/QC analyses.

4.2 Sampling Subsurface Soils

Subsurface soil sampling is conducted to estimate the mean concentrations of contaminants in each source at a site for comparison to inhalation and migration to ground water SSLs. Measurements of soil properties and estimates of the area and depth of contamination in each source are also needed to calculate SSLs for these pathways. Table 31 shows the steps in the DQO process necessary to develop a sampling strategy to meet these objectives. Each of these steps is described below.

4.2.1 State the Problem. Contaminants present in subsurface soils at the site may pose significant risk to human health and the environment through the inhalation of volatiles or by the migration of contaminants through soils to an underlying potable aquifer. The problem is to identify the contaminants and source areas that do not pose significant risk to human health through either of these exposure pathways so that future investigations may be focused on areas and contaminants of true concern.

Site-specific activities in this step include identifying the data collection planning team (including technical experts and key stakeholders) and specifying the available resources (i.e., the cost and time available for sampling). The list of technical experts and stakeholders should contain all key personnel who are involved with applying SSLs to the site. Other activities include developing the conceptual site model and identifying exposure scenarios, which are fully addressed in the *Soil Screening Guidance: User's Guide* (U.S. EPA, 1996).

4.2.2 Identify the Decision. The decision is to determine whether mean soil concentrations in each source area exceed inhalation or migration to ground water SSLs for specific contaminants. If so, the source area will be investigated further. If not, no further action will be taken under CERCLA.

4.2.3 Identify Inputs to the Decision. Site-specific inputs to the decision include the average contaminant concentrations within each source area and the inhalation and migration ground water SSLs. Calculation of the SSLs for the two pathways of concern also requires site-specific measurements of soil properties (i.e., bulk density, fraction organic carbon content, pH, and soil texture class) and estimates of the areal extent and depth of contamination.

A list of feasible sampling and analytical methods should be assembled during this step. EPA recommends the use of field methods where applicable and appropriate. Verify that Contract Laboratory Program (CLP) methods and field methods for analyzing the samples exist and that the analytical method detection limits or field method detection limits are appropriate for the site-specific or generic SSL. The *Sampler's Guide to the Contract Laboratory Program* (U.S. EPA, 1990) and the *User's Guide to the Contract Laboratory Program* (U.S. EPA, 1991d) contain further information on CLP methods.

Table 31. Soil Screening DQOs for Subsurface Soils

DQO Process Steps	Soil Screening Inputs/Outputs
State the Problem	
Identify scoping team	Site manager and technical experts (e.g., toxicologists, risk assessors, hydrogeologists, statisticians).
Develop conceptual site model (CSM)	CSM development (described in Step 1 of the User's Guide, U.S. EPA, 1996).
Define exposure scenarios	Inhalation of volatiles and migration of contaminants from soil to potable ground water (and plant uptake for certain contaminants).
Specify available resources	Sampling and analysis budget, scheduling constraints, and available personnel.
Write brief summary of contamination problem	Summary of the subsurface soil contamination problem to be investigated at the site.
Identify the Decision	
Identify decision	Do mean soil concentrations for particular contaminants (e.g., contaminants of potential concern) exceed appropriate SSLs?
Identify alternative actions	Eliminate area from further action or study under CERCLA or Plan and conduct further investigation.
Identify Inputs to the Decision	
Identify decision	Volatile inhalation and migration to ground water SSLs for specified contaminants Measurements of subsurface soil contaminant concentration
Define basis for screening	Soil Screening Guidance
Identify analytical methods	Feasible analytical methods (both field and laboratory) consistent with program-level requirements.
Specify the Study Boundaries	
Define geographic areas of field investigation	The entire NPL site (which may include areas beyond facility boundaries), except for any areas with clear evidence that no contamination has occurred.
Define population of interest	Subsurface soils
Define scale of decision making	Sources (areas of contiguous soil contamination, defined by the area and depth of contamination or to the water table, whichever is more shallow).
Subdivide site into decision units	Individual sources delineated (area and depth) using existing information or field measurements (several nearby sources may be combined into a single source).
Define temporal boundaries of study	Temporal constraints on scheduling field visits.
Identify (list) practical constraints	Potential impediments to sample collection, such as access, health, and safety issues.
Develop a Decision Rule	
Specify parameter of interest	Mean soil contaminant concentration in a source (as represented by discrete contaminant concentrations averaged within soil borings).
Specify screening level	SSLs calculated using available parameters and site data (or generic SSLs if site data are unavailable).
Specify "if..., then..." decision rule	If the mean soil concentration exceeds the SSL, then investigate the source further. If the mean soil boring concentration is less than the SSL, then no further investigation is required under CERCLA.

Table 31. (continued)

Specify Limits on Decision Errors	
Define QA/QC goals	CLP precision and bias requirements 10% CLP analyses for field methods
Optimize the Design	
Determine how to estimate mean concentration in a source	For each source, the highest mean soil core concentration (i.e., depth-weighted average of discrete contaminant concentrations within a boring).
Define subsurface sampling strategy by evaluating costs and site-specific conditions	Number of soil borings per source area; number of sampling intervals with depth.
Develop planning documents for the field investigation	Sampling and Analysis Plan (SAP) Quality Assurance Project Plan (QAPjP)

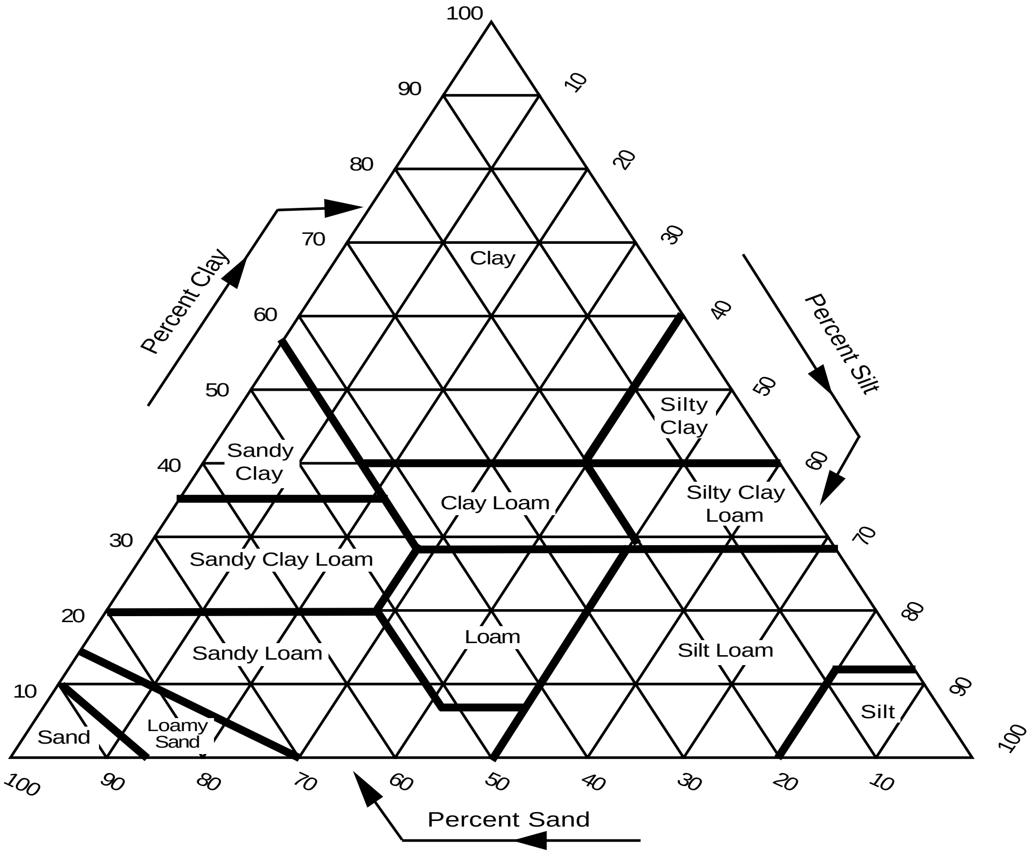
Field methods will be useful in defining the study boundaries (i.e., area and depth of contamination) during site reconnaissance and during the sampling effort. For example, soil gas survey is an ideal method for determining the extent of volatile contamination in the subsurface. EPA expects field methods will become more prevalent and useful because the design and capabilities of field portable instrumentation are rapidly evolving. Documents on standard operating procedures (SOPs) for field methods are available through NTIS and should be referenced in soil screening documentation if these methods are used.

Soil parameters necessary for SSL calculation are soil texture, bulk density, and soil organic carbon. Some of these parameters can be measured in the field, others require laboratory measurement. Although laboratory measurements of these parameters cannot be obtained under the Superfund Contract Laboratory Program, they are readily available from soil testing laboratories across the country.

Note that the size, shape, and orientation of sampling volume (i.e., "support") for heterogenous media have a significant effect on reported measurement values. For instance, particle size has a varying affect on the transport and fate of contaminants in the environment and on the potential receptors. Comparison of data from methods that are based on different supports can be difficult. Defining the sampling support is important in the early stages of site characterization. This may be accomplished through the DQO process with existing knowledge of the site, contamination, and identification of the exposure pathways that need to be characterized. Refer to *Preparation of Soil Sampling Protocols: Sampling Techniques and Strategies* (U.S. EPA, 1992f) for more information about soil sampling support.

Soil Texture. The soil texture class (e.g., loam, sand, silt loam) is necessary to estimate average soil moisture conditions and to estimate infiltration rates. A soil's texture classification is determined from a particle size analysis and the U.S. Department of Agriculture (USDA) soil textural triangle shown at the top of Figure 9. This classification system is based on the USDA soil particle size classification at the bottom of Figure 9. The particle size analysis method in Gee and Bauder (1986) can provide this particle size distribution also. Other particle size analysis methods may be used as long as they provide the same particle size breakpoints for sand/silt (0.05 mm) and silt/clay (0.002 mm). Field methods are an alternative for determining soil textural class; an example from Brady (1990) is also presented in Figure 9.

Figure 9: U.S. Department of Agriculture soil texture classification.



Criteria Used with the Field Method for Determining Soil Texture Classes (Source: Brady, 1990)

Criterion	**Sand**	**Sandy loam**	**Loam**	**Silt loam**	**Clay loam**	**Clay**
1. Individual grains visible to eye	Yes	Yes	Some	Few	No	No
2. Stability of dry clods	Do not form	Do not form	Easily broken	Moderately easily broken	Hard and stable	Very hard and stable
3. Stability of wet clods	Unstable	Slightly stable	Moderately stable	Stable	Very stable	Very stable
4. Stability of "ribbon" when wet soil rubbed between thumb and fingers	Does not form	Does not form	Does not form	Broken appearance	Thin, will break	Very long, flexible

Particle Size, mm

<table>
<tr><td></td><td></td><td>0.002</td><td>0.05</td><td>0.10</td><td>0.25</td><td>0.5</td><td>1.0</td><td>2.0</td></tr>
<tr><td rowspan="2">U.S. Department of Agriculture</td><td rowspan="2">Clay</td><td rowspan="2">Silt</td><td>Very Fine</td><td>Fine</td><td>Med.</td><td>Coarse</td><td>Very Coarse</td><td rowspan="2">Gravel</td></tr>
<tr><td colspan="5">Sand</td></tr>
</table>

Source: USDA.

Dry Bulk Density. Dry soil bulk density (ρ_b) is used to calculate total soil porosity and can be determined for any soil horizon by weighing a thin-walled tube soil sample (e.g., Shelby tube) of known volume and subtracting the tube weight to estimate field bulk density (ASTM D 2937). A moisture content determination (ASTM 2216) is then made on a subsample of the tube sample to adjust field bulk density to dry bulk density. The other methods (e.g., ASTM D 1556, D 2167, D 2922) are not generally applicable to subsurface soils. ASTM soil testing methods are readily available in the *Annual Book of ASTM Standards, Volume 4.08, Soil and Rock; Building Stones*, which is available from ASTM, 100 Barr Harbor Drive, West Conshohocken, PA, 19428.

Organic Carbon and pH. Soil organic carbon is measured by burning off soil carbon in a controlled-temperature oven (Nelson and Sommers, 1982). This parameter is used to determine soil-water partition coefficients from the organic carbon soil-water partition coefficient, K_{oc}. Soil pH is used to select site-specific partition coefficients for metals and ionizing organic compounds (see Part 5). This simple measurement is made with a pH meter in a soil/water slurry (McLean, 1982) and may be measured in the field using a portable pH meter.

4.2.4 Define the Study Boundaries. As discussed in Section 4.1.4, areas that are known to be highly contaminated (i.e., sources) are targeted for subsurface sampling. The information collected on source area and depth is used to calculate site-specific SSLs for the inhalation and migration to ground water pathways. Contamination is defined by the lower of the CLP practical quantitation limit for each contaminant or the SSL. For the purposes of this guidance, source areas are defined by area and depth as contiguous zones of contamination. However, discrete sources that are near each other may be combined and investigated as a single source if site conditions warrant.

4.2.5 Develop a Decision Rule. The decision rule for subsurface soils is:

> If the mean concentration of a contaminant within a source area exceeds the screening level, then investigate that area further.

In this case "screening level" means the SSL. As explained in Section 4.1.5, statistics other than the mean (e.g., the maximum concentration) may be used as estimates of the mean in this comparison as long as they represent valid or conservative estimates of the mean.

4.2.6 Specify Limits on Decision Errors. EPA recognizes that data obtained from sampling and analysis can never be perfectly representative or accurate and that the costs of trying to achieve near-perfect results can outweigh the benefits. Consequently, EPA acknowledges that uncertainty in data must be tolerated to some degree. The DQO process attempts to control the degree to which uncertainty in data affects the outcomes of decisions that are based on data.

The sampling intensity necessary to accurately determine the mean concentration of subsurface soil contamination within a source with a specified level of confidence (e.g., 95 percent) is impracticable for screening due to excessive costs and difficulties with implementation. Therefore, EPA has developed an alternative decision rule based on average concentrations within individual soil cores taken in a source:

> If the mean concentration within **any** soil core taken in a source exceeds the screening level, then investigate that source further.

For each core, the mean core concentration is defined as the depth-weighted average concentration within the zone of contamination (see Section 4.2.7). Since the soil cores are taken in the area(s) of highest contamination within each source, the highest average core concentration among a set of core samples serves as a conservative estimate of the mean source concentration. Because this rule is not a statistical decision, it is not possible to statistically define limits on decision errors.

Standard limits on the precision and bias of sampling and analytical operations conducted during the sampling program do apply. These are specified by the Superfund quality assurance program requirements (U.S. EPA, 1993d), which must be followed during the subsurface sampling effort.

If field methods are used, at least 10 percent of field samples should be split and sent to a CLP laboratory for confirmatory analysis (U.S. EPA, 1993d).

Although the EPA does not require full CLP sample tracking and quality assurance/quality control (QA/QC) procedures for measurement of soil properties, routine EPA QA/QC procedures are recommended, including a Quality Assurance Project Plan (QAPjP), chain-of-custody forms, and duplicate analyses.

4.2.7 Optimize the Design. Within each source, the Soil Screening Guidance suggests taking two to three soil cores using split spoon or Shelby tube samplers. For each soil core, samples should begin at the ground surface and continue at approximately 2-foot intervals until no contamination is encountered or to the water table, whichever is shallower. **Subsurface sampling depths and intervals can be adjusted at a site to accommodate site-specific information on surface and subsurface contaminant distributions and geological conditions** (e.g., large vadose zones in the West).

The number and location of subsurface soil sampling (i.e., soil core) locations should be based on knowledge of likely surface soil contamination patterns and subsurface conditions. This usually means that core samples should be taken directly beneath areas of high surface soil contamination. Surface soils sampling efforts and field measurements (e.g., soil gas surveys) taken during site reconnaissance will provide information on source areas and high contaminant concentrations to help target subsurface sampling efforts. Information in the CSM also will provide information on areas likely to have the highest levels of contamination. Note that there may be sources buried in subsurface soils that are not discernible at the surface. Information on past practices at the site included in the CSM can help identify such areas. Surface geophysical methods also can aid in identifying such areas (e.g., magnetometry to detect buried drums).

The intensity of the subsurface soil sampling needed to implement the soil screening process typically will not be sufficient to fully characterize the extent of subsurface contamination. In these cases, conservative assumptions should be used to develop hypotheses on likely contaminant distributions (e.g., the assumption that soil contamination extends to the water table). Along with knowledge of subsurface hydrogeology and stratigraphy, geostatistics can be a useful tool in developing subsurface contaminant distributions from limited data and can provide information to help guide additional sampling efforts. However, instructions on the use of geostatistics is beyond the scope of this guidance.

Samples for measuring soil parameters should be collected when taking samples for measuring contaminant concentrations. If possible, consider splitting single samples for contaminant and soil parameter measurements. Many soil testing laboratories have provisions in place for handling and testing contaminated samples. However, if testing contaminated samples is a problem, samples may be taken from clean areas of the site as long as they represent the same soil texture and series and are taken from the same depth as the contaminant concentration samples.

The SAP developed for subsurface soils should specify sampling and analytical procedures as well as the development of QA/QC procedures. To identify the appropriate analytical procedures, the screening levels must be known. If data are not available to calculate site-specific SSLs, then the generic SSLs in Appendix A should be used.

Finally, soil investigation for the migration to ground water pathway should not be conducted independently of ground water investigations. Contaminated ground water may indicate the presence of a nearby source area, with contaminants leaching from soil into the aquifer.

4.2.8 Analyzing the Data. The mean soil contaminant concentration for each soil core should be compared to the SSL for the contaminant. The soil core average should be obtained by averaging analyses results for the discrete samples taken along the entire soil core within the zone of contamination (compositing will prevent the evaluation of contaminant concentration trends with depth).

If each subsurface soil core segment represents the same subsurface soil interval (e.g., 2 feet), then the average concentration from the surface to the depth of contamination is the simple arithmetic average of the concentrations measured for core samples representative of each of the 2-foot segments from the surface to the depth of contamination or to the water table. However, if the intervals are not all of the same length (e.g., some are 2 feet while others are 1 foot or 6 inches), then the calculation of the average concentration in the total core must account for the different lengths of the intervals.

If c_i is the concentration measured in a core sample representative of a core interval of length l_i, and the n-th interval is considered to be the last interval in the source area (i.e., the n-th sample represents the depth of contamination), then the average concentration in the core from the surface to the depth of contamination should be calculated as the following depth-weighted average ($\overline{c}$),

$$\overline{c} = \frac{\sum_{i=1}^{n} l_i c_i}{\sum_{i=1}^{n} l_i} \tag{61}$$

If the leach test option is used, a sample representing the average contaminant concentration within the zone of contamination should be formed for each soil core by combining discrete samples into a composite sample for the test. The composites should include only samples taken within the zone of contamination (i.e., clean soil below the lower limit of contamination should not be mixed with contaminated soil).

As with any Superfund sampling effort, all analytical data should be reviewed to ensure that Superfund quality assurance program requirements are met (U.S. EPA, 1993d).

4.2.9 Reporting. The decision process for subsurface soil screening should be thoroughly documented. This documentation should contain as a minimum: a map of the site showing the contaminated soil sources and any areas assumed not to be contaminated, the soil core sampling points within each source, and the soil core sampling points that were compared with the SSLs; the depth and area assumed for each source and their basis; the average soil properties used to calculate

SSLs for each source; a description of how samples were taken and (if applicable) how composite samples were formed; the raw analytical data; the average soil core contaminant concentrations compared with the SSLs for each source; and theresults of all QA/QC analyses.

4.3 Basis for the Surface Soil Sampling Strategies: Technical Analyses Performed

This section describes a series of technical analyses conducted to support the sampling strategy for surface soils outlined in the Soil Screening Guidance. Section 4.3.1 describes the sample design procedure presented in the December 1994 draft guidance (U.S. EAP, 1994h). The remaining sections describe the technical analyses conducted to develop the final SSL sampling strategy. Section 4.3.2 describes an alternative, nonparametric procedure that EPA considered but **rejected** for the soil screening strategy.

Section 4.3.3 describes the simulations conducted to support the selection of the Max test and the Chen test in the final Soil Screening Guidance. These simulation results also can be used to determine sample sizes for site conditions not adequately addressed by the tables in Section 4.1. Quantitation limit and multiple comparison issues are discussed in Sections 4.3.4 and 4.3.5, respectively. Section 4.3.6 describes a limited investigation of compositing samples within individual EA sectors or strata.

4.3.1 1994 Draft Guidance Sampling Strategy. The DQO-based sampling strategy in the 1994 draft Soil Screening Guidance assumed a lognormal distribution for contaminant levels over an EA and derived sample size determinations from lognormal confidence interval procedures by C. E. Land (1971). This section summarizes the rationale for this approach and technical issues raised by peer review.

For the 1994 draft Soil Screening Guidance, EPA based the surface soil SSL methodology on the comparison of the arithmetic mean concentration over an EA with the SSL. As explained in Section 4.1, this approach reflects the type of exposure to soil under a future residential land use scenario. A person moving randomly across a residential lot would be expected to experience an average concentration of contaminants in soil.

Generally speaking, there are few nonparametric approaches to statistical inference about a mean unless a symmetric distribution (e.g., normal) is assumed, in which case the mean and median are identical and inference about the median is the same as inference about the mean. However, environmental contaminant concentration distributions over a surface area tend to be skewed with a long right tail, so symmetry is not plausible. In this case the main options for inference about means are inherently parametric, i.e., they are based on an assumed family of probability distributions.

In addition to being skewed with a long right tail, environmental contaminant concentration data must be positive because concentration measurements cannot be negative. Several standard two-parameter probability models are nonnegative and skewed to the right, including the gamma, lognormal, and Weibull distributions. The properties of these distributions are summarized in Chapter 12 of Gilbert (1987).

The lognormal distribution is the distribution most commonly used for environmental contaminant data (see, e.g., Gilbert, 1987, page 164). The lognormal family can be easy to work with in some respects, due to the work of Land (1971, 1975) on estimating confidence intervals for lognormal parameters, which are also described in Gilbert (1987).

The equation for estimating the Land upper confidence limit (UL) for a lognormal mean has the form

$$UL = \exp\left(\bar{y} + \frac{s_y^2}{2} + \frac{s_y H}{\sqrt{n - 1}} \right) \tag{62}$$

where $\bar{y}$ and s_y are the average and standard deviation of the sample log concentrations. The lower confidence limit (LL) has a similar form. The factor H depends on s_y and n and is tabulated in Gilbert (1987) and Land (1975). If the data truly follow a lognormal distribution, then the Land confidence limits are exact (i.e., the coverage probability of a 95 percent confidence interval is 0.95).

The problem formulation used to develop SSL DQOs in the 1994 draft Soil Screening Guidance tested the null hypothesis H_0: $\mu \geq 2$ SSL versus the alternative hypothesis H_1: $\mu < 2$ SSL, with a Type I error rate of 0.05 (at 2 SSL), and a Type II error rate of 0.20 at 0.5 SSL (μ represents the true EA mean). That is, the probability of incorrectly deciding not to investigate further when the true mean is 2 SSL was set not to exceed 0.05, and the probability of incorrectly deciding to investigate further when the true mean is 0.5 SSL was not to exceed 0.20.

This null hypothesis can be tested at the 5 percent level of significance by calculating Land's upper 95 percent confidence limit for a lognormal mean, if one assumes that the true EA concentrations are lognormally distributed. The null hypothesis is rejected if the upper confidence limit falls below 2 SSL.

Simulation studies of the Land procedure were used to obtain sample size estimates that achieve these DQOs for different possible values of the standard deviation of log concentrations. Additional simulation studies were conducted to calculate sample sizes and to investigate the properties of the Land procedure in situations where specimens are composited.

All of these simulation studies assumed a lognormal distribution of site concentrations. If the underlying site distribution is lognormal, then the composites, viewed as physical averages, are not lognormal (although they may be approximately lognormal). Hence, correction factors are necessary to apply the Land procedure with compositing, if the individual specimen concentrations are assumed lognormal. The correction factors were also developed through simulations. The correction factors are multiplied by the sample standard deviation, s_y, before calculating the confidence limit and conducting the test.

Procedures for estimating sample sizes and testing hypotheses about the site mean using the Land procedure, with and without compositing, are described in the 1994 draft Technical Background Document (U.S. EPA, 1994i).

A peer review of the draft Technical Background Document identified several issues of concern:

- The use of a procedure relying strongly on the assumption of a lognormal distribution
- Quantitation limit issues
- Issues associated with multiple hypothesis tests where multiple contaminants are present in site soils.

The first issue is of concern because the small sample sizes appropriate for surface soil screening will not provide sufficient data to validate this assumption. To address this issue, EPA considered several alternative approaches and performed extensive analyses. These analyses are described in Sections 4.3.2 and 4.3.3. Section 4.3.3 describes extensive simulation studies involving a variety of distributions that were done to compare the Land, Chen, and Max tests and to develop the latter two as options for soil screening.

4.3.2 Test of Proportion Exceeding a Threshold. One of the difficulties noted for the Land test, described in Section 4.3.1, is its strong reliance on an assumption of lognormality (see Section 4.3.3). Even in cases where the assumption may hold, there will rarely be sufficient information to test it.

A second criticism of applying the Land test (or another test based on estimating the mean) is that values must be substituted for values reported as less than a quantitation limit (<QL). (As noted in Section 4.3.4, how one does this substitution is of little relevance if the SSL is much larger than the QL. However, even if a moderate proportion of the data values fall below the QL and are censored, then the lognormal distribution may not be a good model for the observed concentrations.)

A third criticism of using the Land test for screening is its requirement for large sample sizes when the contaminant variability across the EA is expected to be large (e.g., a large coefficient of variation). Because of these drawbacks to applying the Land procedure, EPA considered alternative, nonparametric procedures. One such alternative that was considered is the test described below.

For a given contaminant, let P represent the proportion of all possible sampling units across the EA for which the concentration exceeds 2 SSL. In essence, P represents the proportion of the EA with true contaminant levels above 2 SSL. A nonparametric test involving P was developed as follows.

Let P_0 be a fixed proportion of interest chosen in such a way that if that proportion (or more) of the EA has contamination levels above 2 SSL, then that EA should be investigated further. One way to obtain a rough equivalence between the test for a mean greater than 2 SSL and a test involving P is to choose $1-P_0$ to correspond to the percentile of the lognormal distribution at which the mean occurs. One can show that this is equivalent to choosing

$$P_0 = 1 - \Phi\left[0.5\sigma\right] = 1 - \Phi\left[0.5\sqrt{\ln\left(1+CV^2\right)}\right] \qquad \textbf{(63)}$$

where

σ = assumed standard deviation of the logarithms of the concentrations
CV = assumed coefficient of variation of the contaminant concentrations
Φ = distribution function of the standard normal distribution.

Here, the fixed proportion P_0 will be less than one-half. The hypotheses are framed as

H_0: $P \geq P_0$ (EA needs further investigation)

versus

H_1: $P < P_0$ (EA does not need further investigation).

The test is based on concentration data from a grid sample of N points in the EA (without compositing). Let p represent the proportion of these n points with observed concentrations greater than or equal to 2 SSL. The test is carried out by choosing a critical value, p_c, to meet the desired Type I error rate, that is,

$$\alpha = \text{Prob}\ (p < p_c \mid P = P_0) = 0.05. \qquad \textbf{(64)}$$

The sample size should be chosen to satisfy the Type II error rate at some specified alternative value P_1, where $P_1 < P_0$. For example, to have an 80 percent power at P_1:

$$1 - \beta = \text{Prob}\ (p < p_c \mid P = P_1) = 0.80. \qquad \textbf{(65)}$$

If the same type of rationale for choosing P_0 (corresponding to 2 SSL) is used to make P_1 correspond to 0.5 SSL, then one would choose

$$P_1 = 1 - \Phi\ [0.5\ \sigma + 1.386/\sigma]. \qquad \textbf{(66)}$$

Sample sizes for this test were developed based on the preceding formulation and were found to be approximately the same as those required by the Land procedure, though they tended to be slightly higher than the Land sample sizes for small σ, and slightly smaller for large σ.

The major advantage of this test, in contrast to the Land procedure, for example, is its generality; the only assumption required is that random sampling be used to select the sample points. Its principal disadvantages are:

- Compositing of samples cannot be included (since the calculation of p requires the count of the number of units with observed levels at or above 2 SSL).
- The test does not deal directly with the mean contaminant level at the EA, which is the fundamental parameter for risk calculations.
- Because the test does not depend directly on the magnitude of the concentrations, it is possible that the test will give misleading results relative to a test based on a mean. This can occur, for example, when only a small portion of the EA has very high levels (i.e., a hot spot). In that case, the observed p will converge for increasing n to that proportion of the EA that is contaminated; it would do the same if the concentration levels in that same portion were just slightly above 2 SSL. A test based on a mean for large samples, however, is able to distinguish between these two situations; by its very nature, a test based on a proportion of measurements exceeding a single threshold level cannot.

For these reasons, the test described here based on the proportion of observations exceeding 2 SSL was not selected for inclusion in the current guidance.

4.3.3 Relative Performance of Land, Max, and Chen Tests. A simulation study was conducted to compare the Land, Chen, and Max tests and to determine sample sizes necessary to achieve DQOs. This section describes the design of the simulation study and summarizes its results. Detailed output from the simulations is presented in Appendix I.

Treatment of Data Below the Quantitation Limit. Review of quantitation limits for 110 chemicals showed that for more than 90 percent of the chemicals, the quantitation limit was less than 1 percent of the ingestion SSL. In such cases, the treatment of values below the QL is not expected to have much effect, as long as all data are used in the analysis, with concentrations assigned to results below the QL in some reasonable way. In the simulations, the QL was assumed to be SSL/100 and any simulated value below the QL was set equal to 0.5 QL. This is a conservative assumption based on the comparison of ingestion SSLs with QLs.

Decision Rules. For the **Land procedure**, as discussed in Section 4.3.1, the null hypothesis H_0: $\mu \geq 2$ SSL (where μ represents the true mean concentration for the EA) can be tested at the 5 percent level by calculating Land's upper 95 percent confidence limit for a lognormal mean. The null hypothesis is rejected (i.e., surface soil contaminant concentrations are less than 2 SSL), if this upper confidence limit falls below 2 SSL. This application of the Land (1971) procedure, as described in the draft 1994 Guidance, will be referred to as the "SSL DQOs" and the "original Land procedure."

For the **Max test**, one decides to walk away if the maximum concentration observed in composite samples taken from the EA does not exceed 2 SSL. As indicated in Section 4.1.6, it is viewed as providing a test of the original null hypothesis, H_0: $\mu \geq 2$ SSL. The Max test does not inherently control either type of error rate (i.e., its critical region is always the region below 2 SSL, not where concentrations below a threshold that achieve a specified Type I error rate). However, control of error rates for the Max test can be achieved through the DQO process by choice of design (i.e., by choice of the number N of composite samples and choice of the number C of specimens per composite).

The **Chen test** requires that the null hypothesis have the form H_0: $\mu \leq \mu_0$, with the alternative hypothesis as H_1: $\mu > \mu_0$ (Chen, 1995). Hypotheses or DQOs of this form are referred to as "flipped hypotheses" or "flipped DQOs" because they represent the inverse of the actual hypothesis for SSL decisions. In the simulations, the Chen method was applied with $\mu_0 = 0.5$ SSL at significance levels (Type I error rates) of 0.4, 0.3, 0.2, 0.1, 0.05, 0.025, and 0.01. In this formulation, a Type I error occurs if one decides incorrectly to investigate further when the true site mean, μ, is at or below 0.5 SSL.

The two formulations of the hypotheses are equivalent in the sense that both allow achievement of soil screening DQOs. That is, working with either formulation, it is possible to control the probability of incorrectly deciding to walk away when the true site mean is 2 SSL and to also control the probability of incorrectly deciding to investigate further when the true site mean is 0.5 SSL.

In addition to the original Land procedure, the Chen test, and the Max test, the simulations also include the Land test of the flipped null hypothesis H_0: $\mu \leq 0.5$ SSL at the 10 percent significance level. This Land test of the flipped hypothesis was included to investigate how interchanging the null and alternative hypotheses affected sample sizes for the Land and Chen procedures.

Simulation Distributions. In the following description of the simulations, parameter acronyms used as labels in the tables of results are indicated by capital letters enclosed in parentheses.

Each distribution used for simulation is a mixture of a lower concentration distribution and a higher concentration distribution. The lower distribution represents the EA in its natural (unpolluted) state, and the higher distribution represents contaminated areas. Typically, all measurements of pollutants in uncontaminated areas are below the QL. Accordingly, the lower distribution is assumed to be completely below the QL. For the purposes of this analysis, it is unnecessary to specify any other aspect of the lower distribution, because any measurement below the QL is set equal to 0.5 QL.

A parameter between 0 and 1, called the mixing proportion (MIX), specifies the probability allocated to the lower distribution. The remaining probability (1-MIX) is spread over higher values according to either a lognormal, gamma, or Weibull distribution. The parameters of the higher distribution are chosen so that the overall mixture has a given true EA mean (MU) and a given coefficient of variation (CV). Where s is the sample standard deviation, $\bar{x}$ is the sample mean, and C is the number of specimens per composite sample, CV is defined as:

$$CV = \frac{s}{\bar{x}} \text{ or } CV = \frac{\left(\sqrt{C}\right)s}{\bar{x}}.$$

The following parameter values were used in the simulations:

EA mean (MU) = 0.5 SSL or 2 SSL

EA coefficient of variation (CV) = 1, 1.5, 2, 2.5, 3, 3.5, 4, 5, or 6 (i.e., 100 to 600 percent)

Number of specimens per composite (C) = 1, 2, 3, 4, 5, 6, 8, 9, 12, or 16

Number of composites chemically analyzed (N) = 4, 5, 6, 7, 8, 9, 12, or 16.

The true EA mean was set equal to 0.5 SSL or 2 SSL in order to estimate the two error rates of primary concern. Most CVs encountered in practice probably will lie between 1 and 2.5 (i.e., variability between 100 and 250 percent). This expectation is based on data from the Hanford site (see Hardin and Gilbert, 1993) and the Piazza Road site (discussed in Section 4.3.6). EPA believes that the most practical choices for the number of specimens per composite will be four and six. In some cases, compositing may not be appropriate (the case C = 1 corresponds to no compositing). EPA also believes that for soil screening, a practical number of samples chemically analyzed per EA lies below nine, and that screening decisions about soils in each EA should not be based on fewer than four chemical analyses.

For a given CV, there is a theoretical limit to how large the mixing proportion can be. The values of the mixing proportion used in the simulations are shown below as a function of CV. The case MIX = 0 corresponds to an EA characterized by a gamma, lognormal, or Weibull distribution. A value of MIX near 1 indicates an EA where all concentrations are below the QL except those in a small portion of the EA. Neither of these extremes implies an extreme overall mean. If MIX = 0, the contaminating (higher) distribution can have a low mean, resulting in a low overall mean. If MIX is near 1 (i.e., a relatively small contamination area), a high overall mean can be obtained if the mean of the distribution of contaminant concentrations is high enough.

CV	Values of MIX used in the simulations
1.0	0, 0.49
1.5	0, 0.50
2.0	0, 0.50, 0.75
2.5	0, 0.50, 0.85
3.0	0, 0.50, 0.85
3.5	0, 0.50, 0.90
4.0	0, 0.50, 0.90
5.0	0, 0.50, 0.95
6.0	0, 0.50, 0.95

Treatment of Measurement Error. Measurement errors were assumed to be normally distributed with mean 0 (i.e., unbiased measurements) and standard deviation equal to 20 percent of the true value for each chemically analyzed sample. (Earlier simulations included measurement error standard deviations of 10 percent and 25 percent. The difference in results between these two cases was negligible.)

Number of Simulated Samples. Unique combinations of the simulation parameters considered (i.e., 2 values of the EA mean, 10 values for the number of specimens per composite, 8 values for the number of composite samples, 25 combinations of CV and MIX, and 3 contamination models—lognormal, gamma, Weibull), result in a total of 12,000 simulation conditions. One thousand simulated random samples were generated for each of the 12,000 cases obtained by varying the simulation parameters as described above. The average number of physical samples simulated from an EA for a hypothesis test (i.e., the product CN) was 56.

The following 10 hypothesis tests were applied to each of the 12 million random samples:

- Chen test at significance levels of 0.4, 0.3, 0.2, 0.1, 0.05, 0.025, and 0.01
- Original Land test of the null hypothesis H_0: $\mu \geq 2$ SSL at the 5 percent significance level
- Land test of the flipped null hypothesis H_0: $\mu \leq 0.5$ SSL at the 10 percent significance level
- Maximum test.

These simulations involved generation of approximately 650 million random numbers.

Simulation Results. A complete listing of the simulation results, with 150 columns and 59 lines per page, requires 180 pages and is available from EPA on a 3.5-inch diskette.

Representative results for gamma contamination data, with eight composite samples that each consist of six specimens, are shown in Table 32. The gamma contamination model is recommended for determining sample size requirements because it was consistently seen to be least favorable, in the sense that it required higher sample sizes to achieve DQOs than either of the lognormal or Weibull models. Hence, sample sizes sufficient to protect against a gamma distribution of contaminant concentrations are also protective against a lognormal or Weibull distribution.

Table 32. Comparison of Error Rates for Max Test, Chen Test (at .20 and .10 Significance Levels), and Original Land Test, Using 8 Composites of 6 Samples Each, for Gamma Contamination Data

MU/SSL	MIX	Max test	0.20 Chen test	0.10 Chen test	Land test
C=6 N=8 CV=4					
0.5	.00	.35	.18	.09	.99
0.5	.50	.40	.22	.11	.99
0.5	.90	.40	.19	.09	.98
2.0	.00	.06	.10	.18	.00
2.0	.50	.06	.11	.18	.00
2.0	.90	.04	.16	.29	.01
C=6 N=8 CV=3					
0.5	.00	.24	.18	.10	.93
0.5	.50	.25	.19	.10	.94
0.5	.85	.23	.22	.11	.99
2.0	.00	.04	.03	.06	.00
2.0	.50	.03	.03	.05	.00
2.0	.85	.03	.06	.12	.00
C=6 N=8 CV=2					
0.5	.00	.07	.22	.11	.57
0.5	.50	.06	.19	.09	.68
0.5	.75	.04	.19	.10	.85
2.0	.00	.02	.00	.00	.01
2.0	.50	.02	.00	.01	.00
2.0	.75	.01	.00	.01	.00
C=6 N=8 CV=1					
0.5	.00	.00	.20	.10	.01
0.5	.49	.00	.20	.12	.12
2.0	.00	.01	.00	.00	.02
2.0	.49	.01	.00	.00	.00

MU = True EA Mean - see subsection entitled “Simulation Distributions” in Section 4.3.3.
MIX = Mixing Proportion - see subsection entitled “Simulation Distributions” in Section 4.3.3
C = Number of specimens in a composite.
N = Number of composites analyzed.
CV = EA coefficient of variation $\frac{(\sqrt{C})s}{\bar{x}}$

where s = sample standard deviation and $\bar{x}$ = mean sample concentration

Table 32 shows that the original Land method is unable to control the error rates at 0.5 SSL for gamma distributions. This limitation of the Land method was seen consistently throughout the results for all nonlognormal distributions tested. This limitation led to removal of the Land procedure from the Soil Screening Guidance.

Earlier simulation results for gamma and Weibull distributions did not censor results below the QL and used pure unmixed distributions. In these cases, as the sample size N increased, with all other factors fixed, the Land error rates at 0.5 SSL increased toward 1. Normally, the expectation is that as the sample size increases, information increases, and error rates decrease.

When using data from a Weibull or gamma distribution, the Land confidence interval endpoints converge to a value **that does not equal** the true site mean, μ_x , and results in an increase in error rates. This phenomenon is easily demonstrated, as follows. Let X denote the concentration random variable, let Y = ln(X) denote its logarithm. Let μ_y and σ_y denote the mean and standard deviation of logarithms of the soil concentrations. Then, as the sample size increases, the Land confidence interval endpoints (UL and LL) converge to

$$UL = LL = \exp\left(\mu_y + \frac{\sigma_y^2}{2}\right) . \qquad \textbf{(67)}$$

If X is lognormally distributed, this expression is the mean of X. If X has a Weibull or gamma distribution, this expression is **not** the mean of X. This inconsistency accounts for the increase in error rates with sample size.

Table 32 also shows the fundamental difference between the Max test and the Chen test. For the Max test, the probability of error in deciding to walk away when the EA mean is 2.0 SSL is fairly stable, ranging from 0.01 to 0.06 across the different values of the CV. On the other hand, these error rates vary more across the CV values for the Chen test (e.g., from 0.00 to 0.29 for Chen test at the 0.10 significance level). This occurs because the Chen test is designed to control the other type of error rate (at 0.5 SSL). The Max test is presented in the 1995 Soil Screening Guidance (U.S. EPA, 1995c) because of its simplicity and the stability of its control over the error rate at 2 SSL.

Table 33 shows error rate estimates for four to nine composite samples that each consist of four, six, or eight specimens for EAs with CVs of 2, 2.5, 3, or 3.5, and assuming a gamma distribution. Table 33 should be adequate for most SSL planning purposes. However, more complete simulation results are reported in Appendix I.

Planning for CVs at least as large as 2 is recommended because it is known that CVs greater than 2 occur in practice (e.g., for two of seven EAs in the Piazza Road simulations reported in Section 4.3.6). One conclusion that can be drawn from Table 33 is that composite sample sizes of four are often inadequate. Further support for this conclusion is reported in the Piazza Road simulations discussed in Section 4.3.6.

Conclusions. The primary conclusions from the simulations are:

- For distributions other than lognormal, the Land procedure is prone to decide to investigate further at 0.5 SSL, when the correct decision is to walk away. It is therefore unsuitable for surface soil screening.
- Both the Max test and the Chen test perform acceptably under a variety of distributional assumptions and are potentially suitable for surface soil screening.

Table 33. Error Rates of Max Test and Chen Test at .2 (C20) and .1 (C10) Significance Level for CV = 2, 2.5, 3, 3.5

		CV = 2.0			CV = 2.5			CV = 3.0			CV = 3.5		
N	**MU/SSL**	**Max**	**C20**	**C10**	**Max**	**C20**	**C10**	**Max**	**C20**	**C10**	**Max**	**C20**	**C10**
C = 4													
4	0.5	.09	.20	.11	.14	.18	.09	.19	.18	.08	.24	.20	.10
4	2.0	.13	.08	.16	.19	.17	.28	.20	.21	.33	.26	.29	.42
5	0.5	.11	.21	.10	.15	.18	.09	.26	.20	.08	.26	.20	.09
5	2.0	.10	.05	.11	.10	.09	.18	.17	.19	.30	.18	.23	.36
6	0.5	.11	.21	.12	.21	.20	.10	.28	.21	.11	.31	.19	.09
6	2.0	.06	.03	.08	.08	.08	.14	.11	.13	.23	.11	.18	.28
7	0.5	.12	.20	.10	.25	.22	.11	.31	.20	.09	.36	.18	.10
7	2.0	.04	.03	.05	.05	.04	.09	.08	.11	.18	.08	.14	.23
8	0.5	.16	.19	.09	.25	.20	.09	.36	.20	.10	.42	.20	.09
8	2.0	.02	.02	.03	.04	.03	.07	.05	.08	.14	.07	.13	.21
9	0.5	.16	.21	.11	.28	.20	.09	.36	.18	.09	.44	.22	.12
9	2.0	.01	.01	.02	.03	.03	.06	.04	.07	.13	.07	.12	.20
C = 6													
4	0.5	.03	.20	.12	.08	.21	.12	.15	.20	.10	.16	.17	.08
4	2.0	.14	.03	.08	.16	.08	.17	.17	.14	.24	.20	.19	.33
5	0.5	.04	.20	.10	.11	.17	.09	.17	.20	.10	.22	.20	.10
5	2.0	.09	.02	.05	.09	.04	.10	.13	.10	.18	.15	.13	.24
6	0.5	.06	.20	.11	.14	.21	.10	.19	.20	.10	.25	.20	.10
6	2.0	.04	.01	.02	.06	.03	.07	.09	.07	.14	.09	.10	.19
7	0.5	.06	.20	.09	.12	.19	.10	.23	.22	.10	.29	.21	.10
7	2.0	.02	.00	.01	.05	.02	.04	.06	.06	.10	.08	.09	.14
8	0.5	.06	.19	.09	.15	.20	.10	.25	.19	.10	.30	.19	.10
8	2.0	.02	.00	.01	.02	.01	.03	.03	.03	.05	.04	.06	.11
9	0.5	.06	.20	.10	.18	.22	.11	.28	.20	.11	.34	.19	.09
9	2.0	.01	.00	.01	.02	.01	.02	.03	.02	.04	.03	.05	.09
C = 8													
4	0.5	.02	.21	.13	.06	.19	.10	.10	.21	.10	.14	.18	.08
4	2.0	.12	.02	.05	.15	.04	.09	.17	.09	.17	.19	.14	.25
5	0.5	.03	.22	.11	.05	.20	.11	.11	.20	.10	.17	.19	.09
5	2.0	.07	.01	.02	.09	.02	.06	.09	.04	.10	.12	.08	.17
6	0.5	.02	.18	.09	.08	.21	.11	.13	.19	.10	.20	.20	.10
6	2.0	.04	.00	.01	.06	.01	.02	.07	.04	.07	.08	.07	.13
7	0.5	.03	.20	.11	.09	.20	.11	.18	.21	.11	.22	.20	.11
7	2.0	.03	.00	.00	.04	.01	.01	.04	.02	.04	.05	.05	.09
8	0.5	.04	.20	.10	.11	.21	.11	.17	.21	.10	.26	.19	.10
8	2.0	.02	.00	.00	.02	.01	.01	.04	.01	.03	.03	.03	.06
9	0.5	.04	.21	.11	.11	.21	.10	.20	.19	.10	.30	.23	.12
9	2.0	.01	.00	.00	.02	.00	.01	.01	.00	.01	.02	.02	.04

MU = True EA Mean - see subsection entitled “Simulation Distributions” in Section 4.3.3.
MIX= Mixing Proportion - see subsection entitled “Simulation Distributions” in Section 4.3.3
C = Number of specimens in a composite.
N = Number of composites analyzed.
CV = EA coefficient of variation $\frac{(\sqrt{C})s}{\bar{x}}$

where s = sample standard deviation and $\bar{x}$ = mean sample concentration

4.3.4 Treatment of Observations Below the Limit of Quantitation. Test procedures that are based on estimating a mean contaminant level for an EA, such as the Land and Chen procedures, make use of each measured concentration value. For this reason, the use of all reported concentration measurements in such calculations should be considered regardless of their magnitude—that is, even if the measured levels fall below a quantitation level. One argument for this approach is that the QL is itself an estimate. Another is that some value will have to be substituted for any censored data point (i.e., a point reported as <QL), and the actual measured value is at least as accurate as a substituted value.

The peer review of the Draft Soil Screening Guidance raised the following issue:

> If such censored values do occur in a data set, what values should be used?

There is a substantial amount of literature on this subject and a variety of sophisticated approaches. In the context of SSLs, however, a simple approach is recommended. Consistent with general Superfund guidance, each observation reported as "<QL" shall be replaced with 0.5 QL for computation of the sample mean.

The evidence suggests that the ingestion SSL generally will be 2 orders of magnitude or more greater than the QL for most contaminants. In these cases, the results of soil screening will be insensitive to alternative procedures that could be used to substitute values for observations reported as "<QL." When the SSL is not much greater than the QL (e.g., SSL < 50 QL), the outcome of the soil screening could be affected by the procedure used to substitute for "<QL" values.

The most conservative approach would be to substitute the concentration represented by the QL itself for all observations reported as "<QL." In the context of the SSLs, however, the simple approach of using 0.5 QL is suggested. This will be sufficiently conservative given the conservative factors underlying the SSLs.

4.3.5 Multiple Hypothesis Testing Considerations. The Soil Screening Guidance addresses the following hypothesis testing problem for each EA:

> H_0: mean concentration of a given chemical ≥ 2 SSL

versus

> H_1: mean concentration of a given chemical < 2 SSL.

The default value for the probability of a Type I error is $\alpha = 0.05$, while the default value for the power of the test at 0.5 SSL is $1-\beta = 0.80$. The test is applied separately for each chemical, so that these probabilities apply for each individual chemical. Thus, there is an 80 percent probability of walking away from an EA (i.e., rejecting H_0) when only one chemical is being tested and its true mean level is 0.5 SSL and a 5 percent probability of walking away if its true mean level is 2 SSL.

However, the Soil Screening Guidance does not explicitly address the following issues:

> What is the composite probability of walking away from an EA if there are multiple contaminants?

and

> If such probabilities are unacceptable, how should one compensate when testing for multiple contaminants within a single EA?

The answer to the first question cannot be determined, in general, since the concentrations of the various contaminants will often be dependent on one another (e.g., this would be expected if they originated from the same source of contamination). The joint probability of walking away can be determined, however, if one makes the simplifying assumption that the contaminant concentrations for the different chemicals are independent (uncorrelated). In that case, the probability of walking away is simply the product of the individual rejection probabilities.

For two chemicals (Chemical A and Chemical B, say), this is:

Pr{walking away from EA} = Pr{reject H_0 for Chemical A} × Pr{reject H_0 for Chemical B}.

While these joint probabilities must be regarded as approximate, they nevertheless serve to illustrate the effect on the error rates when dealing with multiple contaminants.

Assume (for illustrative purposes only) that the probabilities for rejecting the null hypothesis (walking away from the EA) for each single chemical appear as follows:

True concentration	Probability of rejecting H_0
0.2 SSL	0.95
0.5 SSL	0.80 (default 1-ß)
0.7 SSL	0.60
1.0 SSL	0.50
1.5 SSL	0.20
2.0 SSL	0.05 (default α)

Let C(A) denote the concentration of Chemical A divided by the SSL, and let P(A) denote the corresponding probability of rejecting H_0. Define C(B) and P(B) similarly for Chemical B. Assuming independence, the joint probabilities of rejecting the null hypothesis (walking away) are as shown in Table 34.

Table 34. Probability of "Walking Away" from an EA When Comparing Two Chemicals to SSLs

Chemical A		**Chemical B**					
C(A)	**P(A)**	**C(B) = 0.2 P(B) =.95**	**C(B) = 0.5 P(B) = .80**	**C(B) = 0.7 P(B) = .60**	**C(B) = 1.0 P(B) = .50**	**C(B) = 1.5 P(B) = .20**	**C(B) = 2.0 P(B) = .05**
0.2	0.95	0.90	0.76	0.57	0.48	0.19	0.05
0.5	0.80	0.76	0.64	0.48	0.40	0.16	0.04
0.7	0.60	0.57	0.48	0.36	0.30	0.12	0.03
1.0	0.50	0.48	0.40	0.30	0.25	0.10	0.03
1.5	0.20	0.19	0.16	0.12	0.10	0.04	0.01
2.0	0.05	0.05	0.04	0.03	0.03	0.01	<0.01

These probabilities demonstrate that the test procedure will tend to be very conservative if multiple chemicals are involved—that is, **all** of the chemical concentrations must be quite low relative to their SSL in order to have a high probability of walking away from the EA. On the other hand, there will be a high probability that further investigation will be called for if the mean concentration for even a single chemical is twice the SSL.

A potential problem occurs when there are several chemicals under consideration and when all or most of them have levels slightly below the SSL (e.g., near 0.5 SSL). For instance, if each of six independent chemicals had levels at 0.5 SSL, the probability of rejecting the null hypothesis would be 80 percent for each such chemical, but the probability of walking away from the EA would be only $(0.80)^6 = 0.26$.

If the same samples are being analyzed for multiple chemicals, then the original choice for the number of such samples ideally should have been based on the worst case (i.e., the chemical expected to have the largest variability). In this case, the probability of correctly rejecting the null hypothesis at 0.5 SSL for the chemicals with less variability will be higher. The overall probability of walking away will be greater than shown above if all or some of the chemicals have less variability than assumed as the basis for determining sample sizes. Here, the sample size will be large enough for the probability of rejecting the null hypothesis at 0.5 SSL to be greater than 0.80 for these chemicals.

The probability values assumed above for deciding that no further investigation is necessary for individual chemicals, which are the basis for these conclusions, are equally applicable for the Land, Chen, and Max tests. They simply represent six hypothetical points of the power curves for these tests (from 0.2 SSL to 2.0 SSL). Therefore, the conclusions are equally applicable for each of the hypothesis testing procedures that have been considered in the current guidance for screening surface soils.

If the surface soil concentrations are positively correlated, as expected when dealing with multiple chemicals, then it is likely that either all the chemicals of concern have relatively high concentrations or they all have relatively low concentrations. In this case, the probability of making the correct decision for an EA would be greater than that suggested by the above calculations that assume independence of the various chemicals.

However, the potential problem of several chemicals having concentrations near 0.5 SSL is not precluded by assuming positive correlations. In fact, it suggests that if the EA average for one chemical is near 0.5 SSL, then the average for others is also likely to be near 0.5 SSL, which is exactly the situation where the probability of **not** walking away from the EA can become large because there is a high probability that H_0 will be rejected for at least one of these chemicals.

An alternative would be to use multiple hypothesis testing procedures to control the overall error rate for the set of chemicals (i.e., the set of hypothesis tests) rather than the separate error rates for the individual chemicals. Guidance for performing multiple hypothesis tests is beyond the scope of the current document. Obtain the advice of a statistician familiar with multiple hypothesis testing procedures if the overall error rates for multiple chemicals is of concern for a particular site. The classical statistical guidance regarding this subject is *Simultaneous Statistical Inference* (Miller, 1991).

4.3.6 Investigation of Compositing Within EA Sectors. If one decides that an EA needs further investigation, then it is natural to inquire which portion(s) of the EA exceed the screening level. This is a different question than simply asking whether or not the EA average soil concentration exceeds the SSL. Conceivably, this question may require additional sampling, chemical analysis, and statistical analysis. A natural question is whether this additional effort can be avoided by forming composites within sectors (subareas) of the EA. The sector with the highest estimated concentration would then be a natural place to begin a detailed investigation.

The simulations to investigate the performance of rules to decide whether further investigation is required, reported in Section 4.3.3, make specific assumptions about the sampling design. It is assumed that N composite samples are chemically analyzed, each consisting of C specimens selected to be statistically representative of the entire EA. The key point, in addition to random sampling, is that composites must be formed **across** sectors rather than **within** sectors. This assumption is necessary to achieve composite samples that are representative of the EA mean (i.e., have the EA mean as their expected value).

If compositing is limited to sectors, such as quadrants, then each composite represents its sector, rather than the entire EA. The simulations reported in Section 4.3.3, and sample sizes based on them, do not apply to this type of compositing. This does not necessarily preclude compositing within sectors for both purposes, i.e., to test the hypothesis about the EA mean and also to indicate the most contaminated sector. However, little is known about the statistical properties of this approach when applying the Max test, which would depend on specifics of the actual spatial distribution of contaminants for a given EA. Because of the lack of extensive spatial data sets for contaminated soil, there is limited basis for determining what sample sizes would be adequate for achieving desired DQOs for various sites. However, one spatial data set was available and used to investigate the performance of compositing within sectors at one site.

Piazza Road Simulations. Data from the Piazza Road NPL site were used to investigate the properties of tests of the EA mean based on compositing within sectors, as compared to compositing between sectors. The investigation of a single site cannot be used to validate a given procedure, but it may indicate whether further investigation of the procedure is worthwhile.

Seven nonoverlapping 0.4-acre EAs were defined within the Piazza Road site. Each EA is an 8-by-12 grid composed of 14'x14' squares. The data consist of a single dioxin measurement of a composite sample from each small square. These measurements are regarded as true values for the simulations reported in this section. Measurement error was incorporated in the same fashion as for the simulations reported in Section 4.3.3.

Each of the seven EAs was subdivided into four 4-by-6 sectors, six 4-by-4 sectors, eight 4-by-3 sectors, twelve 2-by-4 sectors, and sixteen 2-by-3 sectors. Results are presented here for the cases of four, six, and eight sectors because composites of more than eight specimens are expected to be used rarely, if at all.

Table 35 presents the "true" mean and CV for each EA, computed from all 96 measurements within the 0.4-acre EA. The CVs range from 1.0 to 2.2. Note that two of the seven CVs equal or exceed 2 at this site. This supports EPA's belief that at many sites it is prudent, when planning sample size requirements for screening, to assume a CV of at least 2.5 and to consider the possibility of CVs as large as 3 or 3.5.

As data on variability within EAs for different sites and contaminant conditions accrue over time, it will be possible to base the choice of procedures on a larger, more comprehensive database, rather than just a single site.

Appendix J contains results of simulations from the seven Piazza Road EAs. Sampling with replacement from each sector was used, because this was felt to be more consistent with the planned compositing. To estimate the error rates at 0.5 SSL and 2 SSL for each EA, the SSL was defined so that the site mean first was regarded as 0.5 SSL and then was regarded as 2 SSL.

Notation for Results from Piazza Road Simulations. The following notation is used in Appendix J. The design variable (DES) indicates whether compositing was within sector (DES=W) or across sectors (DES=X). As in Section 4.3.3, C denotes the number of specimens per composite, and N denotes the number of composite samples chemically analyzed. Results in Appendix J are for the Chen test at the 10 percent significance level and for the Max test. The true mean and CV are shown in the header for each EA.

Table 35. Means and CVs for Dioxin Concentrations for 7 Piazza Road Exposure Areas

EA	Mean of EA	CV of EA	N
1	2.1	1.0	96
2	2.4	1.6	96
3	5.1	1.1	96
4	4.0	1.2	96
5	9.3	2.0	96
6	15.8	2.2	96
7	2.8	1.4	96

Results and Conclusions from Piazza Road Simulations. Although the results from a single site cannot be assumed to apply to all sites, the following observations can be made based on the Piazza Road simulations reported in Appendix J.

- The error rate at 0.5 SSL for the Chen test, using compositing across sectors (DES=X), is generally close to the nominal rate of 0.10. For compositing within sectors (DES=W), the error rate for Chen at 0.5 SSL is generally much lower than the nominal rate.

- Except for plans involving only four analyses (N = 4), the error rate at 2 SSL is always below 0.05 for the Chen test. For the Max test, the error rate at 2 SSL fluctuated between 0 and 16 percent. The error rate at 2 SSL is smaller for the Chen test at the 10 percent significance level than for the Max test in virtually all cases. The only two exceptions to this are for compositing within sector (DES=W) in EA No. 6.

- This observation provides further support for the conclusion drawn from the simulations reported in Section 4.3.3: plans involving only four analyses can result in high error rates in determining the mean contaminant concentration of an EA with the Max test. In most cases the error rates of concern to EPA (at 2 SSL) are 0.10 or larger.

- In general, error rates estimated from Piazza Road simulations for compositing across sectors are at least as small as would be predicted on the basis of the simulation results reported in Section 4.3.3.

- The simulation results show that compositing within sectors using the Max test may be an option for site managers who want to know whether one sector of an EA is more contaminated than the other. However, use of the Max test when compositing within sectors may lead the site manager to draw conclusions about the mean contaminant concentration in that sector only, not across the entire EA.

Part 5: CHEMICAL-SPECIFIC PARAMETERS

Chemical-specific parameters required for calculating soil screening levels include the organic carbon normalized soil-water partition coefficient for organic compounds (K_{oc}), the soil-water partition coefficient for inorganic constituents (K_d), water solubility (S), Henry's law constant (HLC, H′), air diffusivity ($D_{i,a}$), and water diffusivity ($D_{i,w}$). In addition, the octanol-water partition coefficient (K_{ow}) is needed to calculate K_{oc} values. This part of the background document describes the collection and compilation of these parameters for the SSL chemicals.

With the exception of values for air diffusivity ($D_{i,a}$), water diffusivity ($D_{i,w}$), and certain K_{oc} values, all of the values used in the development of SSLs can be found in the Superfund Chemical Data Matrix (SCDM). SCDM is a computer code that includes more than 25 datafiles containing specific chemical parameters used to calculate factor and benchmark values for the Hazard Ranking System (HRS). Because SCDM datafiles are regularly updated, the user should consult the most recent version of SCDM to ensure that the values are up to date.

5.1 Solubility, Henry's Law Constant, and K_{ow}

Chemical-specific values for solubility, Henry's law constant (HLC), and K_{ow} were obtained from SCDM. In the selection of the value for SCDM, measured or analytical values are favored over calculated values. However, in the event that a measured value is not available, calculated values are used. Table 36 presents the solubility, Henry's law constant, and K_{ow} values taken from SCDM and used to calculate SSLs.

Henry's law constant values were available for all but two of the constituents of interest. Henry's law constants could not be obtained from the SCDM datafiles for either carbazole or mercury. As a consequence, this parameter was calculated according to the following equation:

$$HLC = (VP)(M)/(S) \qquad \textbf{(68)}$$

where

HLC = Henry's law constant (atm-m^3/mol)
VP = vapor pressure (atm)
M = molecular weight (g/mol)
S = solubility (mg/L or g/m^3).

The SSL equations require the dimensionless form of Henry's law constant, or H', which is calculated from HLC (atm-m^3/mol) by multiplying by 41 (U.S. EPA, 1991b). The values taken from SCDM for HLC and the calculated dimensionless values for H' are both presented in Table 36.

5.2 Air ($D_{i,a}$) and Water ($D_{i,w}$) Diffusivities

Few published diffusivities were available for the subject chemicals for air ($D_{i,a}$) and water ($D_{i,w}$). Water and air diffusivities were obtained from the CHEMDAT8 model chemical properties database (DATATWO.WK1). For chemicals not in CHEMDAT8, diffusivities were estimated using the

WATER8 model correlations for air and water diffusivities. Both CHEMDAT8 and WATER8 can be obtained from EPA's SCRAM bulletin board system, as described in Section 3.1.2. Table 37 presents the values used to calculate SSLs.

Table 36. Chemical-Specific Properties Used in SSL Calculations

CAS No.	Compound	S (mg/L)	HLC (atm-m^3/mol)	H′ (dimensionless)	$\log K_{ow}$
83-32-9	Acenaphthene	4.24E+00	1.55E-04	6.36E-03	3.92
67-64-1	Acetone	1.00E+06	3.88E-05	1.59E-03	-0.24
309-00-2	Aldrin	1.80E-01	1.70E-04	6.97E-03	6.50
120-12-7	Anthracene	4.34E-02	6.50E-05	2.67E-03	4.55
56-55-3	Benz(*a*)anthracene	9.40E-03	3.35E-06	1.37E-04	5.70
71-43-2	Benzene	1.75E+03	5.55E-03	2.28E-01	2.13
205-99-2	Benzo(*b*)fluoranthene	1.50E-03	1.11E-04	4.55E-03	6.20
207-08-9	Benzo(*k*)fluoranthene	8.00E-04	8.29E-07	3.40E-05	6.20
65-85-0	Benzoic acid	3.50E+03	1.54E-06	6.31E-05	1.86
50-32-8	Benzo(*a*)pyrene	1.62E-03	1.13E-06	4.63E-05	6.11
111-44-4	Bis(2-chloroethyl)ether	1.72E+04	1.80E-05	7.38E-04	1.21
117-81-7	Bis(2-ethylhexyl)phthalate	3.40E-01	1.02E-07	4.18E-06	7.30
75-27-4	Bromodichloromethane	6.74E+03	1.60E-03	6.56E-02	2.10
75-25-2	Bromoform	3.10E+03	5.35E-04	2.19E-02	2.35
71-36-3	Butanol	7.40E+04	8.81E-06	3.61E-04	0.85
85-68-7	Butyl benzyl phthalate	2.69E+00	1.26E-06	5.17E-05	4.84
86-74-8	Carbazole	7.48E+00	1.53E-08 [a]	6.26E-07	3.59
75-15-0	Carbon disulfide	1.19E+03	3.03E-02	1.24E+00	2.00
56-23-5	Carbon tetrachloride	7.93E+02	3.04E-02	1.25E+00	2.73
57-74-9	Chlordane	5.60E-02	4.86E-05	1.99E-03	6.32
106-47-8	*p*-Chloroaniline	5.30E+03	3.31E-07	1.36E-05	1.85
108-90-7	Chlorobenzene	4.72E+02	3.70E-03	1.52E-01	2.86
124-48-1	Chlorodibromomethane	2.60E+03	7.83E-04	3.21E-02	2.17
67-66-3	Chloroform	7.92E+03	3.67E-03	1.50E-01	1.92
95-57-8	2-Chlorophenol	2.20E+04	3.91E-04	1.60E-02	2.15
218-01-9	Chrysene	1.60E-03	9.46E-05	3.88E-03	5.70
72-54-8	DDD	9.00E-02	4.00E-06	1.64E-04	6.10
72-55-9	DDE	1.20E-01	2.10E-05	8.61E-04	6.76
50-29-3	DDT	2.50E-02	8.10E-06	3.32E-04	6.53
53-70-3	Dibenz(*a*,*h*)anthracene	2.49E-03	1.47E-08	6.03E-07	6.69
84-74-2	Di-*n*-butyl phthalate	1.12E+01	9.38E-10	3.85E-08	4.61
95-50-1	1,2-Dichlorobenzene	1.56E+02	1.90E-03	7.79E-02	3.43
106-46-7	1,4-Dichlorobenzene	7.38E+01	2.43E-03	9.96E-02	3.42
91-94-1	3,3-Dichlorobenzidine	3.11E+00	4.00E-09	1.64E-07	3.51
75-34-3	1,1-Dichloroethane	5.06E+03	5.62E-03	2.30E-01	1.79

Table 36 (continued)

CAS No.	Compound	S (mg/L)	HLC (atm-m^3/mol)	H′ (dimensionless)	log K_{ow}
107-06-2	1,2-Dichloroethane	8.52E+03	9.79E-04	4.01E-02	1.47
75-35-4	1,1-Dichloroethylene	2.25E+03	2.61E-02	1.07E+00	2.13
156-59-2	*cis*-1,2-Dichloroethylene	3.50E+03	4.08E-03	1.67E-01	1.86
156-60-5	*trans*-1,2-Dichloroethylene	6.30E+03	9.38E-03	3.85E-01	2.07
120-83-2	2,4-Dichlorophenol	4.50E+03	3.16E-06	1.30E-04	3.08
78-87-5	1,2-Dichloropropane	2.80E+03	2.80E-03	1.15E-01	1.97
542-75-6	1,3-Dichloropropene	2.80E+03	1.77E-02	7.26E-01	2.00
60-57-1	Dieldrin	1.95E-01	1.51E-05	6.19E-04	5.37
84-66-2	Diethylphthalate	1.08E+03	4.50E-07	1.85E-05	2.50
105-67-9	2,4-Dimethylphenol	7.87E+03	2.00E-06	8.20E-05	2.36
51-28-5	2,4-Dinitrophenol	2.79E+03	4.43E-07	1.82E-05	1.55
121-14-2	2,4-Dinitrotoluene	2.70E+02	9.26E-08	3.80E-06	2.01
606-20-2	2,6-Dinitrotoluene	1.82E+02	7.47E-07	3.06E-05	1.87
117-84-0	Di-*n*-octyl phthalate	2.00E-02	6.68E-05	2.74E-03	8.06
115-29-7	Endosulfan	5.10E-01	1.12E-05	4.59E-04	4.10
72-20-8	Endrin	2.50E-01	7.52E-06	3.08E-04	5.06
100-41-4	Ethylbenzene	1.69E+02	7.88E-03	3.23E-01	3.14
206-44-0	Fluoranthene	2.06E-01	1.61E-05	6.60E-04	5.12
86-73-7	Fluorene	1.98E+00	6.36E-05	2.61E-03	4.21
76-44-8	Heptachlor	1.80E-01	1.09E-03	4.47E-02	6.26
1024-57-3	Heptachlor epoxide	2.00E-01	9.50E-06	3.90E-04	5.00
118-74-1	Hexachlorobenzene	6.20E+00	1.32E-03	5.41E-02	5.89
87-68-3	Hexachloro-1,3-butadiene	3.23E+00	8.15E-03	3.34E-01	4.81
319-84-6	α-HCH (α-BHC)	2.00E+00	1.06E-05	4.35E-04	3.80
319-85-7	β-HCH (β-BHC)	2.40E-01	7.43E-07	3.05E-05	3.81
58-89-9	γ-HCH (Lindane)	6.80E+00	1.40E-05	5.74E-04	3.73
77-47-4	Hexachlorocyclopentadiene	1.80E+00	2.70E-02	1.11E+00	5.39
67-72-1	Hexachloroethane	5.00E+01	3.89E-03	1.59E-01	4.00
193-39-5	Indeno(1,2,3-*cd*)pyrene	2.20E-05	1.60E-06	6.56E-05	6.65
78-59-1	Isophorone	1.20E+04	6.64E-06	2.72E-04	1.70
7439-97-6	Mercury	---	1.14E-02 [b]	4.67E-01	---
72-43-5	Methoxychlor	4.50E-02	1.58E-05	6.48E-04	5.08
74-83-9	Methyl bromide	1.52E+04	6.24E-03	2.56E-01	1.19
75-09-2	Methylene chloride	1.30E+04	2.19E-03	8.98E-02	1.25
95-48-7	2-Methylphenol	2.60E+04	1.20E-06	4.92E-05	1.99
91-20-3	Naphthalene	3.10E+01	4.83E-04	1.98E-02	3.36
98-95-3	Nitrobenzene	2.09E+03	2.40E-05	9.84E-04	1.84
86-30-6	*N*-Nitrosodiphenylamine	3.51E+01	5.00E-06	2.05E-04	3.16
621-64-7	*N*-Nitrosodi-*n*-propylamine	9.89E+03	2.25E-06	9.23E-05	1.40

Table 36 (continued)

CAS No.	Compound	S (mg/L)	HLC (atm-m^3/mol)	H′ (dimensionless)	log K_{ow}
87-86-5	Pentachlorophenol	1.95E+03	2.44E-08	1.00E-06	5.09
108-95-2	Phenol	8.28E+04	3.97E-07	1.63E-05	1.48
129-00-0	Pyrene	1.35E-01	1.10E-05	4.51E-04	5.11
100-42-5	Styrene	3.10E+02	2.75E-03	1.13E-01	2.94
79-34-5	1,1,2,2-Tetrachloroethane	2.97E+03	3.45E-04	1.41E-02	2.39
127-18-4	Tetrachloroethylene	2.00E+02	1.84E-02	7.54E-01	2.67
108-88-3	Toluene	5.26E+02	6.64E-03	2.72E-01	2.75
8001-35-2	Toxaphene	7.40E-01	6.00E-06	2.46E-04	5.50
120-82-1	1,2,4-Trichlorobenzene	3.00E+02	1.42E-03	5.82E-02	4.01
71-55-6	1,1,1-Trichloroethane	1.33E+03	1.72E-02	7.05E-01	2.48
79-00-5	1,1,2-Trichloroethane	4.42E+03	9.13E-04	3.74E-02	2.05
79-01-6	Trichloroethylene	1.10E+03	1.03E-02	4.22E-01	2.71
95-95-4	2,4,5-Trichlorophenol	1.20E+03	4.33E-06	1.78E-04	3.90
88-06-2	2,4,6-Trichlorophenol	8.00E+02	7.79E-06	3.19E-04	3.70
108-05-4	Vinyl acetate	2.00E+04	5.11E-04	2.10E-02	0.73
75-01-4	Vinyl chloride	2.76E+03	2.70E-02	1.11E+00	1.50
108-38-3	*m*-Xylene	1.61E+02	7.34E-03	3.01E-01	3.20
95-47-6	*o*-Xylene	1.78E+02	5.19E-03	2.13E-01	3.13
106-42-3	*p*-Xylene	1.85E+02	7.66E-03	3.14E-01	3.17

CAS = Chemical Abstracts Service.
S = Solubility in water (20-25 °C).
HLC = Henry's law constant.
H′ = Dimensionless Henry's law constant (HLC [atm-m^3/mol] * 41) (25 °C).
K_{ow} = Octanol/water partition coefficient.

[a] HLC was calculated using the equation: HLC = vapor pressure * molecular wt. / solubility. Vapor pressure is 6.83E-10 atm and molecular weight is 167.21 g/mol for carbazole.

[b] Value from WATER8 model database.

Table 37. Air Diffusivity ($D_{i,a}$) and Water Diffusivity ($D_{i,w}$) Values for SSL Chemicals (25°C)[a]

CAS No.	Compound	$D_{i,a}$ (cm^2/s)	$D_{i,w}$ (cm^2/s)
83-32-9	Acenaphthene	4.21E-02	7.69E-06
67-64-1	Acetone	1.24E-01	1.14E-05
309-00-2	Aldrin	1.32E-02	4.86E-06
120-12-7	Anthracene	3.24E-02	7.74E-06
56-55-3	Benz(*a*)anthracene	5.10E-02	9.00E-06
71-43-2	Benzene	8.80E-02	9.80E-06
205-99-2	Benzo(*b*)fluoranthene	2.26E-02	5.56E-06
207-08-9	Benzo(*k*)fluoranthene	2.26E-02	5.56E-06
65-85-0	Benzoic acid	5.36E-02	7.97E-06
50-32-8	Benzo(*a*)pyrene	4.30E-02	9.00E-06
111-44-4	Bis(2-chloroethyl)ether	6.92E-02	7.53E-06
117-81-7	Bis(2-ethylhexyl)phthalate	3.51E-02	3.66E-06
75-27-4	Bromodichloromethane	2.98E-02	1.06E-05
75-25-2	Bromoform	1.49E-02	1.03E-05
71-36-3	Butanol	8.00E-02	9.30E-06
85-68-7	Butyl benzyl phthalate	1.74E-02 [b]	4.83E-06 [b]
86-74-8	Carbazole	3.90E-02 [b]	7.03E-06 [b]
75-15-0	Carbon disulfide	1.04E-01	1.00E-05
56-23-5	Carbon tetrachloride	7.80E-02	8.80E-06
57-74-9	Chlordane	1.18E-02	4.37E-06
106-47-8	*p*-Chloroaniline	4.83E-02	1.01E-05
108-90-7	Chlorobenzene	7.30E-02	8.70E-06
124-48-1	Chlorodibromomethane	1.96E-02	1.05E-05
67-66-3	Chloroform	1.04E-01	1.00E-05
95-57-8	2-Chlorophenol	5.01E-02	9.46E-06
218-01-9	Chrysene	2.48E-02	6.21E-06
72-54-8	DDD	1.69E-02 [b]	4.76E-06 [b]
72-55-9	DDE	1.44E-02	5.87E-06
50-29-3	DDT	1.37E-02	4.95E-06
53-70-3	Dibenz(*a,h*)anthracene	2.02E-02 [b]	5.18E-06 [b]
84-74-2	Di-*n*-butyl phthalate	4.38E-02	7.86E-06
95-50-1	1,2-Dichlorobenzene	6.90E-02	7.90E-06
106-46-7	1,4-Dichlorobenzene	6.90E-02	7.90E-06
91-94-1	3,3-Dichlorobenzidine	1.94E-02	6.74E-06
75-34-3	1,1-Dichloroethane	7.42E-02	1.05E-05
107-06-2	1,2-Dichloroethane	1.04E-01	9.90E-06
75-35-4	1,1-Dichloroethylene	9.00E-02	1.04E-05
156-59-2	*cis*-1,2-Dichloroethylene	7.36E-02	1.13E-05
156-60-5	*trans*-1,2-Dichloroethylene	7.07E-02	1.19E-05
120-83-2	2,4-Dichlorophenol	3.46E-02	8.77E-06

Table 37 (continued)

CAS No.	Compound	$D_{i,a}$ (cm^2/s)	$D_{i,w}$ (cm^2/s)
78-87-5	1,2-Dichloropropane	7.82E-02	8.73E-06
542-75-6	1,3-Dichloropropene	6.26E-02	1.00E-05
60-57-1	Dieldrin	1.25E-02	4.74E-06
84-66-2	Diethylphthalate	2.56E-02 [b]	6.35E-06 [b]
105-67-9	2,4-Dimethylphenol	5.84E-02	8.69E-06
51-28-5	2,4-Dinitrophenol	2.73E-02	9.06E-06
121-14-2	2,4-Dinitrotoluene	2.03E-01	7.06E-06
606-20-2	2,6-Dinitrotoluene	3.27E-02	7.26E-06
117-84-0	Di-*n*-octyl phthalate	1.51E-02	3.58E-06
115-29-7	Endosulfan	1.15E-02	4.55E-06
72-20-8	Endrin	1.25E-02	4.74E-06
100-41-4	Ethylbenzene	7.50E-02	7.80E-06
206-44-0	Fluoranthene	3.02E-02	6.35E-06
86-73-7	Fluorene	3.63E-02 [b]	7.88E-06 [b]
76-44-8	Heptachlor	1.12E-02	5.69E-06
1024-57-3	Heptachlor epoxide	1.32E-02 [b]	4.23E-06 [b]
118-74-1	Hexachlorobenzene	5.42E-02	5.91E-06
87-68-3	Hexachloro-1,3-butadiene	5.61E-02	6.16E-06
319-84-6	α-HCH (α-BHC)	1.42E-02	7.34E-06
319-85-7	β-HCH (β-BHC)	1.42E-02	7.34E-06
58-89-9	γ-HCH (Lindane)	1.42E-02	7.34E-06
77-47-4	Hexachlorocyclopentadiene	1.61E-02	7.21E-06
67-72-1	Hexachloroethane	2.50E-03	6.80E-06
193-39-5	Indeno(1,2,3-*cd*)pyrene	1.90E-02	5.66E-06
78-59-1	Isophorone	6.23E-02	6.76E-06
7439-97-6	Mercury	3.07E-02 [b]	6.30E-06 [b]
72-43-5	Methoxychlor	1.56E-02	4.46E-06
74-83-9	Methyl bromide	7.28E-02	1.21E-05
75-09-2	Methylene chloride	1.01E-01	1.17E-05
95-48-7	2-Methylphenol	7.40E-02	8.30E-06
91-20-3	Naphthalene	5.90E-02	7.50E-06
98-95-3	Nitrobenzene	7.60E-02	8.60E-06
86-30-6	*N*-Nitrosodiphenylamine	3.12E-02 [b]	6.35E-06 [b]
621-64-7	*N*-Nitrosodi-*n*-propylamine	5.45E-02 [b]	8.17E-06 [b]
87-86-5	Pentachlorophenol	5.60E-02	6.10E-06
108-95-2	Phenol	8.20E-02	9.10E-06
129-00-0	Pyrene	2.72E-02 [b]	7.24E-06 [b]
100-42-5	Styrene	7.10E-02	8.00E-06
79-34-5	1,1,2,2-Tetrachloroethane	7.10E-02	7.90E-06
127-18-4	Tetrachloroethylene	7.20E-02	8.20E-06

Table 37 (continued)

CAS No.	Compound	$D_{i,a}$ (cm²/s)	$D_{i,w}$ (cm²/s)
108-88-3	Toluene	8.70E-02	8.60E-06
8001-35-2	Toxaphene	1.16E-02	4.34E-06
120-82-1	1,2,4-Trichlorobenzene	3.00E-02	8.23E-06
71-55-6	1,1,1-Trichloroethane	7.80E-02	8.80E-06
79-00-5	1,1,2-Trichloroethane	7.80E-02	8.80E-06
79-01-6	Trichloroethylene	7.90E-02	9.10E-06
95-95-4	2,4,5-Trichlorophenol	2.91E-02	7.03E-06
88-06-2	2,4,6-Trichlorophenol	3.18E-02	6.25E-06
108-05-4	Vinyl acetate	8.50E-02	9.20E-06
75-01-4	Vinyl chloride	1.06E-01	1.23E-06
108-38-3	*m*-Xylene	7.00E-02	7.80E-06
95-47-6	*o*-Xylene	8.70E-02	1.00E-05
106-42-3	*p*-Xylene	7.69E-02	8.44E-06

CAS = Chemical Abstracts Service.

[a] Value from CHEMDAT8 model database unless indicated otherwise.

[b] Estimated using correlations in WATER8 model.

5.3 Soil Organic Carbon/Water Partition Coefficients (K_{oc})

Application of SSLs for the inhalation and migration to ground water pathways requires K_{oc} values for each organic chemical of concern. K_{oc} values are also needed for site-specific exposure modeling efforts. An initial review of the literature uncovered significant variability in this parameter, with reported measured values for a compound sometimes varying over several orders of magnitude. This variability can be attributed to several factors, including actual variability due to differences in soil or sediment properties, differences in experimental and analytical approaches used to measure the values, and experimental or measurement error. To resolve this difficulty, an extensive literature review was conducted to uncover all available measured values and to identify approaches and information that might be useful in developing valid K_{oc} values.

The soil-water partitioning behavior of nonionizing and ionizing organic compounds differs because the partitioning of ionizing organics can be significantly influenced by soil pH. For this reason, different approaches were required to estimate K_{oc} values for nonionizing and ionizing organic compounds.

5.3.1 K_{oc} for Nonionizing Organic Compounds. As noted earlier, there is significant variability in reported K_{oc} values and an extensive literature search was conducted to collect all available measured K_{oc} values for the nonionizing hydrophobic organic compounds of interest.

In the literature search, misquotation error was minimized by obtaining the original references whenever possible. Values from compilations and secondary references were used only when the original references could not be obtained. Redundancy of values was avoided, although in rare instances it was not possible to determine if compilations included such values, especially when data were reported as "selected" values.

In certain references, soil-water partition coefficients (e.g., K_d or K_p) were reported along with the organic carbon content of the soil. In these cases, K_{oc} was computed by dividing K_d by the fractional soil organic carbon content (f_{oc}, g/g). If the partition coefficient was normalized to soil organic matter (i.e., K_{om}), it was converted to K_{oc} as follows (Dragun, 1988):

$$K_{oc} = 1.724\ K_{om} \tag{69}$$

where

1.724 = conversion factor from organic matter to organic carbon ($f_{om} = 1.724\ f_{oc}$)
K_{om} = partition coefficient normalized to organic matter (L/kg)
f_{om} = fraction organic matter (g/g).

Once collected, K_{oc} values were reviewed. It was not possible to systematically evaluate each source for accuracy or consistency or to analyze sources of variability between references because of wide variations in soil and sediment properties, experimental and analytical methods, and the manner in which these were reported in each reference. This, and the limited number of K_{oc} values for many compounds, prevented any meaningful statistical analysis to eliminate outliers.

Collected values were qualitatively reviewed, however, and some values were excluded. Values measured for low-carbon-content sorbents (i.e., $f_{oc} \le 0.001$) are generally beyond the range of the linear relationship between soil organic carbon and K_d and were rejected in most cases. Some references produced consistently high or low values and, as a result, were eliminated. Values were also eliminated if they fell outside the range of other measured values. The final values used are presented in Appendix K along with their reference sources.

Summary statistics for the measured K_{oc} values are presented in Table 38. The geometric mean of the K_{oc} for each nonionizing organic compound is used as the the central tendency K_{oc} value because it is a more suitable estimate of the central tendency of a distribution of environmental values with wide variability.

The data contained in Table 38 are summarized in Table 39 for each of the nonionizing organic compounds for which measured K_{oc} values were available. As shown, measured values are available for only a subset of the SSL compounds. As a consequence, an alternative methodology was applied to determine K_{oc} values for the entire set of nonionizing hydrophobic organic compounds of interest.

It has long been noted that a strong linear relationship exists between K_{oc} and K_{ow} (octanol/water partition coefficient) (Lyman et al., 1982) and that this relationship can be used to predict K_{oc} in the absence of measured data. One such relationship was reported by Di Toro (1985). This relationship was selected for use in calculating K_{oc} values for most semivolatile nonionizing organic compounds (Group 1 in Table 39) because it considers particle interaction and was shown to be in conformity with observations for a large set of adsorption-desorption data (Di Toro, 1985). Di Toro's equation is as follows:

$$\log K_{oc} = 0.00028 + (0.983 \times \log K_{ow}) \tag{70}$$

For volatile organic compounds (VOCs), Equation 70 consistently overpredicted K_{oc} values when compared to measured data. For this reason, a separate regression equation was developed using log K_{ow} and measured log K_{oc} values for VOCs, chlorinated benzenes, and certain chlorinated pesticides:

$$\log K_{oc} = 0.0784 + (0.7919 \times \log K_{ow}) \qquad \textbf{(71)}$$

Equation 71 was developed from a linear regression calculated at the 95 percent confidence level. The correlation coefficient (r) was 0.99 with an r^2 of 0.97. The compounds and data used to develop this equation are provided in Appendix K. Equation 71 was used to calculate K_{oc} values for VOCs, chlorobenzenes, and certain chlorinated pesticides (i.e., Group 2 in Table 39). Log K_{oc} values calculated using Equations 70 and 71 were rounded to two decimal places, and the resulting K_{oc} values were rounded to two decimal places in scientific notation (i.e, as they appear in Table 39) prior to calculating SSLs.

Table 38. Summary Statistics for Measured K_{oc} Values: Nonionizing Organics[a]

	K_{oc} (L/kg)				
Compound	**Geometric Mean**	**Average**	**Minimum**	**Maximum**	**Sample Size**
Acenaphthene	4,898	5,028	3,890	6,166	2
Aldrin	48,685	48,686	48,394	48,978	2
Anthracene	23,493	24,362	14,500	33,884	9
Benz(*a*)anthracene	357,537	459,882	150,000	840,000	4
Benzene	62	66	31	100	13
Benzo(*a*)pyrene	968,774	1,166,733	478,947	2,130,000	3
Bis(2-chloroethyl)ether	76	76	76	76	1
Bis(2-ethylhexyl)phthalate	111,123	114,337	87,420	141,254	2
Bromoform	126	126	126	126	1
Butyl benzyl phthalate	13,746	14,055	11,128	16,981	2
Carbon tetrachloride	152	158	123	224	3
Chlordane	51,310	51,798	44,711	58,884	2
Chlorobenzene	224	260	83	500	9
Chloroform	53	57	28	81	5
DDD	45,800	45,800	45,800	45,800	1
DDE	86,405	86,405	86,405	86,405	1
DDT	677,934	792,158	285,467	1,741,516	6
Dibenz(a,h)anthracene	1,789,101	2,029,435	565,014	3,059,425	14
1,2-Dichlorobenzene (*o*)	379	390	267	529	9
1,4-Dichlorobenzene (*p*)	616	687	273	1,375	16
1,1-Dichloroethane	53	54	46	62	2
1,2-Dichloroethane	38	44	22	76	3
1,1-Dichloroethylene	65	65	65	65	1

Table 38 (continued)

	K_{oc} (L/kg)				
Compound	**Geometric Mean**	**Average**	**Minimum**	**Maximum**	**Sample Size**
trans-1,2-Dichloroethylene	38	38	38	38	1
1,2-Dichloropropane	47	47	47	47	1
1,3-Dichloropropene	27	27	24	32	3
Dieldrin	25,546	25,604	23,308	27,399	3
Diethylphthalate	82	84	69	98	2
Di-*n*-butylphthalate	1,567	1,580	1,384	1,775	2
Endosulfan	2,040	2,040	2,040	2,040	1
Endrin	10,811	11,422	7,724	15,885	4
Ethylbenzene	204	207	165	255	5
Fluoranthene	49,096	49,433	41,687	54,954	3
Fluorene	7,707	8,906	3,989	16,218	6
Heptachlor	9,528	10,070	6,810	13,330	2
Hexachlorobenzene	80,000	80,000	80,000	80,000	1
α-HCH (α-BHC)	1,762	1,835	1,022	2,891	12
β-HCH (β-BHC)	2,139	2,241	1,156	3,563	14
γ-HCH (Lindane)	1,352	1,477	731	3,249	65
Methoxychlor	80,000	80,000	80,000	80,000	1
Methyl bromide	9	9	9	9	1
Methyl chloride	6	6	6	6	1
Methylene chloride	10	10	10	10	1
Naphthalene	1,191	1,231	830	1,950	20
Nitrobenzene	119	141	31	270	10
Pentachlorobenzene	32,148	36,114	11,381	55,176	5
Pyrene	67,992	70,808	43,807	133,590	27
Styrene	912	912	912	912	1
1,1,2,2-Tetrachloroethane	79	79	79	79	1
Tetrachloroethylene	265	272	177	373	15
Toluene	140	145	94	247	12
Toxaphene	95,816	95,816	95,816	95,816	1
1,2,4-Trichlorobenzene	1,659	1,783	864	3,125	17
1,1,1-Trichloroethane	135	139	106	179	5
1,1,2-Trichloroethane	75	77	60	108	4
Trichloroethylene	94	97	57	150	21
o-Xylene	241	241	222	258	4
m-Xylene	196	204	158	289	3
p-Xylene	311	313	260	347	3

[a] See Appendix K for sources of measured values.

Table 39. Comparison of Measured and Calculated K_{oc} Values

CAS No.	Compound	Chemical Group [a]	Log K_{ow}	Log K_{oc} (L/kg)	Calculated K_{oc} (L/kg)	Measured K_{oc} (L/kg)
83-32-9	Acenaphthene	1	3.92	3.85	7.08E+03	4.90E+03
67-64-1	Acetone	1	-0.24	-0.24	5.75E-01	---
309-00-2	Aldrin	1	6.50	6.39	2.45E+06	4.87E+04
120-12-7	Anthracene	1	4.55	4.47	2.95E+04	2.35E+04
56-55-3	Benz(*a*)anthracene	1	5.70	5.60	3.98E+05	3.58E+05
71-43-2	Benzene	2	2.13	1.77	5.89E+01	6.17E+01
205-99-2	Benzo(*b*)fluoranthene	1	6.20	6.09	1.23E+06	---
207-08-9	Benzo(*k*)fluoranthene	1	6.20	6.09	1.23E+06	---
50-32-8	Benzo(*a*)pyrene	1	6.11	6.01	1.02E+06	9.69E+05
111-44-4	Bis(2-chloroethyl)ether	1	1.21	1.19	1.55E+01	7.59E+01
117-81-7	Bis(2-ethylhexyl)phthalate	1	7.30	7.18	1.51E+07	1.11E+05
75-27-4	Bromodichloromethane	2	2.10	1.74	5.50E+01	---
75-25-2	Bromoform	2	2.35	1.94	8.71E+01	1.26E+02
71-36-3	Butanol	1	0.85	0.84	6.92E+00	---
85-68-7	Butyl benzyl phthalate	1	4.84	4.76	5.75E+04	1.37E+04
86-74-8	Carbazole	1	3.59	3.53	3.39E+03	---
75-15-0	Carbon disulfide	2	2.00	1.66	4.57E+01	---
56-23-5	Carbon tetrachloride	2	2.73	2.24	1.74E+02	1.52E+02
57-74-9	Chlordane	2	6.32	5.08	1.20E+05	5.13E+04
106-47-8	*p*-Chloroaniline	1	1.85	1.82	6.61E+01	---
108-90-7	Chlorobenzene	2	2.86	2.34	2.19E+02	2.24E+02
124-48-1	Chlorodibromomethane	2	2.17	1.80	6.31E+01	---
67-66-3	Chloroform	2	1.92	1.60	3.98E+01	5.25E+01
218-01-9	Chrysene	1	5.70	5.60	3.98E+05	---
72-54-8	DDD	1	6.10	6.00	1.00E+06	4.58E+04
72-55-9	DDE	1	6.76	6.65	4.47E+06	8.64E+04
50-29-3	DDT	1	6.53	6.42	2.63E+06	6.78E+05
53-70-3	Dibenz(*a,h*)anthracene	1	6.69	6.58	3.80E+06	1.79E+06
84-74-2	Di-*n*-butyl phthalate	1	4.61	4.53	3.39E+04	1.57E+03
95-50-1	1,2-Dichlorobenzene	2	3.43	2.79	6.17E+02	3.79E+02
106-46-7	1,4-Dichlorobenzene	2	3.42	2.79	6.17E+02	6.16E+02
91-94-1	3,3-Dichlorobenzidine	2	3.51	2.86	7.24E+02	---
75-34-3	1,1-Dichloroethane	2	1.79	1.50	3.16E+01	5.34E+01
107-06-2	1,2-Dichloroethane	2	1.47	1.24	1.74E+01	3.80E+01
75-35-4	1,1-Dichloroethylene	2	2.13	1.77	5.89E+01	6.50E+01
156-59-2	*cis*-1,2-Dichloroethylene	2	1.86	1.55	3.55E+01	---
156-60-5	*trans*-1,2-Dichloroethylene	2	2.07	1.72	5.25E+01	3.80E+01
78-87-5	1,2-Dichloropropane	2	1.97	1.64	4.37E+01	4.70E+01
542-75-6	1,3-Dichloropropene	2	2.00	1.66	4.57E+01	2.71E+01

Table 39 (continued)

CAS No.	Compound	Chemical Group [a]	Log K_{ow}	Log K_{oc} (L/kg)	Calculated K_{oc} (L/kg)	Measured K_{oc} (L/kg)
60-57-1	Dieldrin	2	5.37	4.33	2.14E+04	2.55E+04
84-66-2	Diethylphthalate	1	2.50	2.46	2.88E+02	8.22E+01
105-67-9	2,4-Dimethylphenol	1	2.36	2.32	2.09E+02	---
121-14-2	2,4-Dinitrotoluene	1	2.01	1.98	9.55E+01	---
606-20-2	2,6-Dinitrotoluene	1	1.87	1.84	6.92E+01	---
117-84-0	Di-*n*-octyl phthalate	1	8.06	7.92	8.32E+07	---
115-29-7	Endosulfan	2	4.10	3.33	2.14E+03	2.04E+03
72-20-8	Endrin	2	5.06	4.09	1.23E+04	1.08E+04
100-41-4	Ethylbenzene	2	3.14	2.56	3.63E+02	2.04E+02
206-44-0	Fluoranthene	1	5.12	5.03	1.07E+05	4.91E+04
86-73-7	Fluorene	1	4.21	4.14	1.38E+04	7.71E+03
76-44-8	Heptachlor	1	6.26	6.15	1.41E+06	9.53E+03
1024-57-3	Heptachlor epoxide	1	5.00	4.92	8.32E+04	---
118-74-1	Hexachlorobenzene	2	5.89	4.74	5.50E+04	8.00E+04
87-68-3	Hexachloro-1,3-butadiene	1	4.81	4.73	5.37E+04	---
319-84-6	α-HCH (α-BHC)	2	3.80	3.09	1.23E+03	1.76E+03
319-85-7	β-HCH (β-BHC)	2	3.81	3.10	1.26E+03	2.14E+03
58-89-9	γ-HCH (Lindane)	2	3.73	3.03	1.07E+03	1.35E+03
77-47-4	Hexachlorocyclopentadiene	1	5.39	5.30	2.00E+05	---
67-72-1	Hexachloroethane	2	4.00	3.25	1.78E+03	---
193-39-5	Indeno(1,2,3-*cd*)pyrene	1	6.65	6.54	3.47E+06	---
78-59-1	Isophorone	1	1.70	1.67	4.68E+01	---
72-43-5	Methoxychlor	1	5.08	4.99	9.77E+04	8.00E+04
74-83-9	Methyl bromide	2	1.19	1.02	1.05E+01	9.00E+00
75-09-2	Methylene chloride	2	1.25	1.07	1.17E+01	1.00E+01
95-48-7	2-Methylphenol	1	1.99	1.96	9.12E+01	---
91-20-3	Naphthalene	1	3.36	3.30	2.00E+03	1.19E+03
98-95-3	Nitrobenzene	1	1.84	1.81	6.46E+01	1.19E+02
86-30-6	*N*-Nitrosodiphenylamine	1	3.16	3.11	1.29E+03	---
621-64-7	*N*-Nitrosodi-*n*-propylamine	1	1.40	1.38	2.40E+01	---
1336-36-3	PCBs	1	5.58	5.49	3.09E+05	---
108-95-2	Phenol	1	1.48	1.46	2.88E+01	---
129-00-0	Pyrene	1	5.11	5.02	1.05E+05	6.80E+04
100-42-5	Styrene	1	2.94	2.89	7.76E+02	9.12E+02
79-34-5	1,1,2,2-Tetrachloroethane	2	2.39	1.97	9.33E+01	7.90E+01
127-18-4	Tetrachloroethylene	2	2.67	2.19	1.55E+02	2.65E+02
108-88-3	Toluene	2	2.75	2.26	1.82E+02	1.40E+02
8001-35-2	Toxaphene	1	5.50	5.41	2.57E+05	9.58E+04
120-82-1	1,2,4-Trichlorobenzene	2	4.01	3.25	1.78E+03	1.66E+03

Table 39 (continued)

CAS No.	Compound	Chemical Group [a]	Log K_{ow}	Log K_{oc} (L/kg)	Calculated K_{oc} (L/kg)	Measured K_{oc} (L/kg)
71-55-6	1,1,1-Trichloroethane	2	2.48	2.04	1.10E+02	1.35E+02
79-00-5	1,1,2-Trichloroethane	2	2.05	1.70	5.01E+01	7.50E+01
79-01-6	Trichloroethylene	2	2.71	2.22	1.66E+02	9.43E+01
108-05-4	Vinyl acetate	1	0.73	0.72	5.25E+00	---
75-01-4	Vinyl chloride	2	1.50	1.27	1.86E+01	---
108-38-3	*m*-Xylene	2	3.20	2.61	4.07E+02	1.96E+02
95-47-6	*o*-Xylene	2	3.13	2.56	3.63E+02	2.41E+02
106-42-3	*p*-Xylene	2	3.17	2.59	3.89E+02	3.11E+02

[a] Group 1: log K_{oc} = 0.983 log K_{ow} + 0.00028.

Group 2: (VOCs, chlorobenzenes, and certain chlorinated pesticides) log K_{oc} = 0.7919 log K_{ow} + 0.0784.

Note: Calculated values rounded as shown for subsequent SSL calculations.

5.3.2 K_{oc} for Ionizing Organic Compounds. Sorption models used to describe the behavior of nonionizing hydrophobic organic compounds in the natural environment are not appropriate for predicting the partitioning of ionizable organic compounds. Certain organic compounds such as amines, carboxylic acids, and phenols contain functional groups that ionize under subsurface pH conditions (Schellenberg et al., 1984). Because the ionized and the neutral species of such compounds have different sorption coefficients, sorption models based solely on the partitioning of the neutral species may not accurately predict soil sorption under different pH conditions.

To address this problem, a technique was employed to predict K_{oc} values for the 15 ionizing SSL organic compounds over the pH range of the subsurface environment. These compounds include:

Organic Acids

- Benzoic acid
- 2-Chlorophenol
- 2,4-Dichlorophenol
- 2,4-Dimethylphenol
- 2,4-Dinitrophenol
- 2-Methylphenol
- Pentachlorophenol
- Phenol
- 2,3,4,5-Tetrachlorophenol
- 2,3,4,6-Tetrachlorophenol
- 2,4,5-Trichlorophenol
- 2,4,6-Trichlorophenol

Organic Bases

- *p*-Chloroaniline
- *N*-Nitrosodiphenylamine
- *N*-Nitrosodi-*n*-propylamine

Estimation of K_{oc} values for these chemicals involves two analyses. First, the extent to which the compound ionizes under subsurface conditions must be determined to estimate the relative proportion of neutral and ionized species under the conditions of concern. Second, the K_{oc} values for the neutral and ionized forms ($K_{oc,n}$ and $K_{oc,i}$) must be determined and weighted according to the extent of ionization at a particular pH to estimate a pH-specific K_{oc} value. For organic acids, the ionized species is an anion (A^-) with a lower tendency to sorb to subsurface materials than the neutral species. Therefore, $K_{oc,i}$ for organic acids is likely to be less than $K_{oc,n}$. In the case of organic bases, the ionized species is positively charged (HB^+) so that $K_{oc,i}$ is likely to be greater than $K_{oc,n}$.

It should be noted that this approach is based on the assumption that the sorption of ionizing organic compounds to soil is similar to hydrophobic organic sorption in that the dominant sorbent is soil organic carbon. Shimizu et al. (1993) demonstrated that, for several "natural solids," pentachlorophenol sorption correlates more strongly with cation exchange capacity and clay content than with organic carbon content. This suggests that this organic acid interacts more strongly with soil mineral constituents than organic carbon. The estimates of K_{oc} developed here may overpredict contaminant mobility because they ignore potential sorption to soil components other than organic carbon.

Extent of Ionization. The sorption potential of ionized and neutral species differs because most subsurface solids (i.e., soil and aquifer materials) have a negative net surface charge. Therefore, positively charged chemicals have a greater tendency to sorb than neutral forms, and neutral species sorb more readily than negatively charged forms. Thus, predictions for the total sorption of any ionizable organic compound must consider the extent to which it ionizes over the range of subsurface pH conditions of interest. Consistent with the EPA/Office of Solid Waste (EPA/OSW) Hazardous Waste Identification Rule (HWIR) proposal (U.S. EPA, 1992a), the 7.5th, 50th, and 92.5th percentiles (i.e., pH values of 4.9, 6.8, and 8.0) for 24,921 field-measured ground water pH values in the U.S. EPA STORET database are defined as the pH conditions of interest for SSL development.

The extent of ionization can be viewed as the fraction of neutral species present that, for organic acids, can be determined from the following pH-dependent relationship (Lee et al., 1990):

$$\Phi_{n,\mathrm{acid}} = \frac{[HA]}{[HA] + [A^-]} = \left(1 + 10^{\,\mathrm{pH}-\mathrm{pKa}}\right)^{-1} \tag{72}$$

where

$\Phi_{n,acid}$ = fraction of neutral species present for organic acids (unitless)
[HA] = equilibrium concentration of organic acid (mol/L)
$[A^-]$ = equilibrium concentration of anion (mol/L)
pKa = acid dissociation constant (unitless).

Using Equation 68, one can show that, in ground water systems with pH values exceeding the pKa by 1.5 pH units, the ionizing species predominates, and, in ground water systems with pH values that are 1.5 pH units less than the pKa, the neutral species predominates. At pH values approximately equal to the pKa, a mixed system of both neutral and ionizing components occurs.

The fraction of neutral species for organic bases is defined by:

$$\Phi_{n,\mathrm{base}} = \frac{[B^\circ]}{[B^\circ] + [HB^+]} = \left(1 + 10^{\,\mathrm{pKa}-\mathrm{pH}}\right)^{-1} \tag{73}$$

where

$\Phi_{n,base}$ = fraction of neutral species present for organic bases (unitless)
$[B^\circ]$ = equilibrium concentration of neutral organic base (mol/L)
$[HB^+]$ = equilibrium concentration of ionized species (mol/L).

As with organic acids, pH conditions determine the relative concentrations of neutral and ionized species in the system. However, unlike organic acids, the neutral species predominates at pH values that exceed the pKa, and the ionized species predominates at pH values less than the pKa. For the SSL organic bases, *N*-nitrosodi-*n*-propylamine and *N*-nitrosodiphenylamine have very low pKa values and the neutral species are expected to prevail under environmental pH conditions. The pKa for *p*-chloroaniline, however, is 4.0 and, at low subsurface pH conditions (i.e., pH = 4.9), roughly 10 percent of the compound will be present as the less mobile ionized species.

Table 40 presents pKa values and fraction neutral species present over the ground water pH range for the SSL ionizing organic compounds. This table shows that ionized species are significant for only some of the constituents under normal subsurface pH conditions. The pKa values for phenol, 2-methylphenol, and 2,4-dimethylphenol are 9.8 or greater. Hence, the neutral species of these compounds predominates under typical subsurface conditions (i.e., pH = 4.9 to 8), and these compounds will be treated as nonionizing organic compounds (see Section 5.3.1). The pKa value for 2,4-dinitrophenol is less than 4 and the ionized species of this compound predominates under subsurface conditions. However, the pKas for 2-chlorophenol, 2,4-dichlorophenol, 2,4,5-trichlorophenol, 2,4,6-trichlorophenol, 2,3,4,5-tetrachlorophenol, 2,3,4,6-tetrachlorophenol, pentachlorophenol, and benzoic acid fall within the range of environmentally significant pH conditions. Mixed systems consisting of both the neutral and the ionized species will prevail under such conditions with both species contributing to total sorption.

Table 40. Degree of Ionization (Fraction of Neutral Species, Φ) as a Function of pH

Compound	pKa[a]	pH = 4.9	pH = 6.8	pH = 8.0
Benzoic acid	4.18	0.1600	0.0024	0.0002
p-Chloroaniline[b]	4.0	0.8882	0.9984	0.9999
2-Chlorophenol	8.40	0.9997	0.9755	0.7153
2,4-Dichlorophenol	7.90	0.9990	0.9264	0.4427
2,4-Dimethylphenol	10.10	1.0000	0.9995	0.9921
2,4-Dinitrophenol	3.30	0.0245	0.0003	0.00002
2-Methylphenol	9.80	1.0000	0.9990	0.9844
N-Nitrosodiphenylamine[b]	< 0	1.0000	1.0000	1.0000
N-Nitrosodi-*n*-propylamine[b]	< 1	0.9999	1.0000	1.0000
Pentachlorophenol	4.80	0.4427	0.0099	0.0006
Phenol	10.0	1.0000	0.9994	0.9901
2,3,4,5-Tetrachlorophenol	6.35[c]	0.9657	0.2619	0.0219
2,3,4,6-Tetrachlorophenol	5.30	0.7153	0.0307	0.0020
2,4,5-Trichlorophenol	7.10	0.9937	0.6661	0.1118
2,4,6-Trichlorophenol	6.40	0.9693	0.2847	0.0245

[a] Kollig et al. (1993).

[b] Denotes that the compound is an organic base.

[c] Lee et al. (1991).

Prediction of Soil-Water Partition Coefficients. Lee et al. (1990) developed a relationship from thermodynamic equilibrium considerations to predict the total sorption of an ionizable organic compound from the partitioning of its ionized and neutral forms:

$$K_{oc} = K_{oc,n}\Phi_n + K_{oc,i}\,(1 - \Phi_n) \qquad \textbf{(74)}$$

where

K_{oc} = soil organic carbon/water partition coefficient (L/kg)
$K_{oc,n}$ = partition coefficient for the neutral species (L/kg)
Φ_n = fraction of neutral species present for acids or bases
$K_{oc,i}$ = partition coefficient for the ionized species (L/kg).

This relationship defines the total sorption coefficient for any ionizing compound as the sum of the weighted individual sorption coefficients for the ionized and neutral species at a given pH. Lee et al. (1990) verified that this relationship adequately predicts laboratory-measured K_{oc} values for pentachlorophenol.

A literature review was conducted to compile the pKa and the laboratory-measured values of $K_{oc,n}$ and $K_{oc,i}$ shown in Table 41. Data collected during this review are presented in RTI (1994), along with the references reviewed. Sorption coefficients for both neutral and ionized species were reported for only four of the nine ionizable organic compounds of interest. Sorption coefficients reported for the remaining compounds were generally $K_{oc,n}$, and estimates of $K_{oc,i}$ were necessary to predict the compound's total sorption. The methods for estimating $K_{oc,i}$ for organic acids and organic bases are discussed separately in the following subsections.

Organic Acids. Sorption coefficients for both the neutral and ionized species have been reported for two chlorophenolic compounds: 2,4,6-trichlorophenol and pentachlorophenol. For 2,4,5-trichlorophenol and 2,3,4,5-tetrachlorophenol, soil-water partitioning coefficient (K_p) data in the literature were adequate to allow calculation of $K_{oc,i}$ from K_p and soil f_{oc} (Lee et al., 1991). From these measured values, the ratios of $K_{oc,i}$ to $K_{oc,n}$ are: 0.1 (2,4,6-trichlorophenol), 0.02 (pentachlorophenol), 0.015 (2,4,5-trichlorophenol), and 0.051 (2,3,4,5-tetrachlorophenol). A ratio of 0.015 (1.5 percent) was selected as a conservative value to estimate $K_{oc,i}$ for the remaining phenolic compounds, benzoic acid, and vinyl acetate.

Organic Bases. No measured sorption coefficients for either the neutral or the ionized species were found for the three organic bases of interest (*N*-nitrosodi-*n*-propylamine, *N*-nitrosodiphenylamine, and *p*-chloroaniline). Generally, the sorption of ionizable organic bases has not been as well investigated as that of the organic acids, and there has been no relationship developed between the sorption coefficients of the neutral and ionized species. EPA is currently initiating research on models for predicting the sorption of organic bases in the subsurface.

As noted earlier, the neutral species of the organic base predominates at pH values exceeding the pKa. For *N*-nitrosodi-*n*-propylamine (pKa < 1) and *N*-nitrosodiphenylamine (pKa < 0), the neutral species is present under environmentally significant conditions. The neutral species constitutes approximately 90 percent of the system for *p*-chloroaniline (Table 40).

Table 41. Soil Organic Carbon/Water Partition Coefficients and pKa Values for Ionizing Organic Compounds

Compound	$K_{oc,n}$ (L/kg)	$K_{oc,i}$ (L/kg)	pKa[a]
Benzoic acid	32[b]	0.5[c]	4.18
2-Chlorophenol	398[b]	6.0[c]	8.40
2,4-Dichlorophenol	159[d]	2.4[c]	7.90
2,4-Dinitrophenol	0.8[a]	0.01[c]	3.30
Pentachlorophenol	19,953[e]	398[e]	4.80
2,3,4,5-Tetrachlorophenol	17,916[f]	67[g]	6.35[h]
2,3,4,6-Tetrachlorophenol	6,190[i]	93[c]	5.30
2,4,5-Trichlorophenol	2,380[i]	36[j]	7.10
2,4,6-Trichlorophenol	1,070[i]	107[k]	6.40

[a] Kollig et al. (1993).

[b] Meylan et al. (1992).

[c] Estimate based on the ratio of $K_{oc,i}/K_{oc,n}$ for compounds for which data exist; $K_{oc,i}$ was estimated to be 0.015 × $K_{oc,n}$.

[d] Calculated using data ($K_p = 0.62$, $f_{oc} = 0.0039$) contained in Lee et al. (1991); agrees well with Boyd (1982) reporting measured K_{oc} = 126 L/kg.

[e] Lee et al. (1990).

[f] Average of values reported for two aquifer materials from Schellenberg et al. (1984).

[g] Calculated using data ($K_p = 0.26$, $f_{oc} = 0.0039$) contained in Lee et al. (1991).

[h] Lee et al. (1991).

[i] Schellenberg et al. (1984).

[j] Calculated using data ($K_p = 0.14$, $f_{oc} = 0.0039$) contained in Lee et al. (1991).

[k] Kukowski (1989).

The neutral species has a lower tendency to sorb to subsurface materials than the positively charged ionized species. As a consequence, the determination of overall sorption potential based solely on the neutral species for *N*-nitrosodi-*n*-propylamine, *N*-nitrosodiphenylamine, and *p*-chloroaniline is conservative, and these three organic bases will be treated as nonionizing organic compounds (see Section 5.3.1).

Soil-Water Partition Coefficients for Ionizing Organic Compounds. Partition coefficients for the neutral and ionized species ($K_{oc,n}$ and $K_{oc,i}$, respectively) and pKa values for nine ionizable organic compounds are provided in Table 41. These parameters can be used in Equation 74 to compute K_{oc} values for organic acids at any given pH. K_{oc} values for each of the ionizable compounds of interest are presented in Table 42 for pHs of 4.9, 6.8, and 8.0. Appendix L contains pH-specific K_{oc} values for ionizable organics over this entire range.

5.4 Soil-Water Distribution Coefficients (K_d) for Inorganic Constituents

As with organic chemicals, development of SSLs for inorganic chemicals (i.e., toxic metals) requires a soil-water partition coefficient (K_d) for each constituent. However, the simple relationship between soil organic carbon content and sorption observed for organic chemicals does not apply to inorganic constituents. The soil-water distribution coefficient (K_d) for metals and other inorganic compounds is affected by numerous geochemical parameters and processes, including pH; sorption to clays, organic matter, iron oxides, and other soil constituents; oxidation/reduction conditions; major ion chemistry; and the chemical form of the metal. The number of significant influencing parameters, their variability in the field, and differences in experimental methods result in as much as seven orders of magnitude variability in measured metal K_d values reported in the literature (Table 43). This variability makes it much more difficult to derive generic K_d values for metals than for organics.

Table 42. Predicted Soil Organic Carbon/Water Partition Coefficients (K_{oc},L/kg) as a Function of pH: Ionizing Organics

Compound	pH = 4.9	pH = 6.8	pH = 8.0
Benzoic acid	5.5	0.6	0.5
2-Chlorophenol	398	388	286
2,4-Dichlorophenol	159	147	72
2,4-Dinitrophenol	0.03	0.01	0.01
Pentachlorophenol	9,055	592	410
2,3,4,5-Tetrachlorophenol	17,304	4,742	458
2,3,4,6-Tetrachlorophenol	4,454	280	105
2,4,5-Trichlorophenol	2,365	1,597	298
2,4,6-Trichlorophenol	1,040	381	131

Because of their great variability and a limited number of data points, no meaningful estimate of central tendency K_d values for metals could be derived from available measured values. For this reason, an equilibrium geochemical speciation model (MINTEQ) was selected as the best approach for estimating K_d values for the variety of environmental conditions expected to be present at Superfund sites.

This approach and model were also used by OSW to estimate generic K_d values for metals proposed for use in the HWIR proposal (U.S. EPA, 1992a). The HWIR MINTEQA2 analyses were conducted under a variety of geochemical conditions and metal concentrations representative of solid waste landfills across the Nation. The metal K_d values developed for this effort were reviewed for SSL application and were used as preliminary values to develop the September 1993 draft SSLs.

Upon further review of the HWIR MINTEQ modeling effort, EPA decided it was necessary to conduct a separate MINTEQ modeling effort to develop metal K_d values for SSL application. Reasons for this decision include the following:

- It was necessary to expand the modeling effort to include other metal contaminants likely to be encountered at Superfund sites (i.e., beryllium, copper, and zinc).
- HWIR work incorporated low, medium, and high concentrations of dissolved organic acids that are present in municipal solid waste (MSW) leachate. These organic acids are not expected to exist in high concentrations in pore waters underlying Superfund sites; therefore, their inclusion in the Superfund contaminated soil scenario is not warranted.
- The HWIR modeling simulations for chromium (+3) were found to be in error. This error has been corrected in subsequent HWIR modeling work but corrected results were not available at the time of preliminary SSL development.

Table 43. Summary of Collected K_d Values Reported in Literature

	AECL (1990)[a]	Baes and Sharp (1983) or Baes et al. (1984)[b]			Coughtrey et al. (1985)[c]	Battelle (1989)[d]
Metal	**Range**	**Geometric Mean[e]**	**Range**	**No. Values**	**Range**	**Range**
Antimony	45-550	45[f]	--	--	--	2.0-15.9
Arsenic[e]	--	200[f]	--	--	--	5.86-19.4
Arsenic (+3)	--	3.3[g]	1.0-8.3	19	--	--
Arsenic (+5)	--	6.7[g]	1.9-18	37	--	--
Barium	--	60[f]	--	--	--	530-16,000
Beryllium	250-3,000	650[f]	--	--	--	70-8,000
Cadmium	2.7-17,000	6.4[h]	1.26-26.8	28	32-50	14.9-567
Chromium	1.7-2,517	850[f]	--	--	--	--
Chromium (+2)	--	2,200[g]	470-150,000	15	--	--
Chromium (+3)	--	--	--	--	--	168-3,600
Chromium (+6)	--	37[g]	1.2-1,800	18	--	16.8-360
Mercury[e]	--	10[f]	--	--	--	322-5,280
Nickel	60-4,700	150[f]	--	--	~20	12.2-650
Selenium	150-1,800	300[f]	--	--	< 9	5.9-14.9
Silver	2.7-33,000	46[h]	10-1,000	16	50	0.4-40.0
Thallium	--	1,500[f]	--	--	--	0.0-0.8
Vanadium	--	1,000[f]	--	--	--	50-100.0
Zinc	0.1-100,000	38[h]	0.1-8,000	146	≥ 20	--

[a] The Atomic Energy of Canada, Limited (AECL, 1990) presents the distribution of K_d values according to four major soil types—sand, silt, clay, and organic material. Their data were obtained from available literature.

[b] Baes et al. (1984) present K_d values for approximately 220 agricultural soils in the pH range of 4.5 to 9. Their data were derived from available literature and represent a diverse mixture of soils, extracting solutions, and laboratory techniques.

[c] Coughtrey et al. (1985) report best estimates and ranges of measured soil K_d values for a limited number of metals.

[d] Battelle Memorial Institute (Battelle, 1989) reports a range in K_d values as a function of pH (5 to 9) and sorbent content (a combination of clay, aluminum and iron oxyhydroxides, and organic matter content). The sorbent content ranges were <10 percent, 10 to 30 percent, and >30 percent sorbent. Their data were based on available literature.

[e] The valence of these metals is not reported in the documents.

[f] Estimated based on the correlation between K_d and soil-to-plant concentration factor (B_v).

[g] Average value reported by Baes and Sharp (1983).

[h] Represents the median of the logarithms of the observed values.

For these reasons, a MINTEQ modeling effort was expanded to develop a series of metal-specific isotherms for several of the metals expected to be present in soils underlying Superfund sites. The model used was an updated version of MINTEQA2 obtained from Allison Geoscience Consultants, Inc. Model results are reported in the December 1994 draft Technical Background Document (U.S. EPA, 1994i) and were used to calculate the SSLs presented in the December 1994 draft Soil Screening Guidance (U.S. EPA, 1994h).

The MINTEQA2 model was further updated by Allison Geoscience Consultants, Inc., in 1995 to include thermodynamic data for silver, an improved estimate of water saturation in the vadose zone (i.e., water saturation is assumed to be 77.7 percent saturated as opposed to 100 percent), and revised estimates of sorbent mass (i.e., organic matter content, iron oxide content).

This updated model, which is expected to be made public through EPA's Environmental Research Laboratory in Athens, Georgia, was used to revise the generic K_d values for the EPA/OSW HWIR modeling effort. The metal K_d values for SSL application were also revised. Model results are contained in this document. The following section describes the important assumptions and limitations of this modeling effort.

5.4.1 Modeling Scope and Approach. New MINTEQA2 modeling runs were conducted to develop sorption isotherms for barium, beryllium, cadmium, chromium (+3), copper, mercury (+2), nickel, silver, and zinc. The general approach and input values used for pH, iron oxide (FeOx) concentration, and background chemistry were unchanged from the HWIR modeling effort.

The HWIR MINTEQA2 analyses were conducted under a variety of geochemical conditions and metal concentrations. Three types of parameters were identified as part of the chemical speciation modeling effort: (1) parameters that have a direct first-order impact on metal speciation and are characterized by a wide range in environmental variability; (2) parameters that have an indirect, generally less pronounced effect on metal speciation and are characterized by a relatively small or insignificant environmental variability; and (3) parameters that may have a direct first-order impact on metal speciation but neither the natural variability nor its significance is known.

In the HWIR modeling effort, parameters of the first type ("master variables") were limited to those having a significant effect on model results, including pH, concentration of available amorphous iron oxide adsorption sites (i.e., FeOx content), concentration of solid organic matter adsorption sites (with a dependent concentration of dissolved natural organic matter), and concentration of leachate organic acids expected to be present in MSW leachate. High, medium, and low values were assigned to each of the master variables to account for their natural environmental variability. The SSL modeling effort used this same approach and inputs except that anthropogenic organic acids were not included in the model simulations. Furthermore, the SSL modeling effort incorporated a medium fraction of organic carbon (f_{oc}) that correlated to the HWIR high concentration.

Parameters of the second type constitute the background pore-water chemistry, which consists of chemical constituents commonly occurring in ground water at concentrations great enough to affect metal speciation. These constituents were treated as constants in both the SSL and HWIR effort. The third type of parameter was entirely omitted from consideration in both modeling efforts due to poorly understood geochemistry and the lack of reliable thermodynamic data. The most important of these parameters is the oxidation-reduction (redox) potential. To compensate, both modeling efforts incorporated an approach that was most protective of the environment with respect to the impact of redox potential on the partitioning of redox-sensitive metals (i.e., each metal was modeled in the oxidation state that most enhances metal mobility).

For the HWIR modeling effort, metal concentrations were varied from the maximum contaminant level (MCL) to 1,000 times the MCL for each individual metal. This same approach was taken for SSL modeling, although for certain metals the concentration range was extended to determine the metal concentration at which the sorption isotherm departed from linearity.

Sorption isotherms for arsenic (+3), chromium (+6), selenium, and thallium are unchanged from the previous efforts and are based on laboratory-derived pH-dependent sorption relationships developed for HWIR. Using these relationships, the K_d distribution as a function of pH is presented for each of these four metals in Figure 10.

Sorption isotherms for antimony and vanadium could not be estimated using MINTEQA2 because the thermodynamic databases do not contain the required reactions and associated equilibrium constants. Sufficient experimental research has not been conducted to develop pH-dependent relationships for these two metals. As a consequence, K_d values for antimony and vanadium were obtained from Baes et al. (1984) (Table 43). These K_d values are not pH-dependent.

5.4.2 Input Parameters. Table 44 lists high, medium, and low values for pH and iron oxide used for both the HWIR and SSL MINTEQ modeling efforts. Sources for these values are as follows (U.S. EPA, 1992a):

- Values for pH were obtained from analysis of 24,921 field-measured pH values contained in the EPA STORET database. The pH values of 4.9, 6.8, and 8.0 correspond to the 7.5th, 50th, and 92.5th percentiles of the distribution.
- Iron oxide contents were based on analysis of six aquifer samples collected over a wide geographic area, including Florida, New Jersey, Oregon, Texas, Utah, and Wisconsin. The lowest of the six analyses was taken to be the low value, the average of the six was used as the medium value, and the highest was taken as the high value.

The development of the values presented in Table 44 is described in more detail in U.S. EPA (1992a).

Thirteen chemical constituents commonly occurring in ground water were used to define the background pore-water chemistry for HWIR and SSL modeling efforts (Table 45). Because these constituents were treated as constants, a single total ion concentration, corresponding to the median total metal concentration from a probability distribution obtained from the STORET database, was assigned to each of the background pore-water constituents (U.S. EPA, 1992a).

Although the HWIR and the SSL MINTEQ modeling efforts were consistent in the majority of the assumptions and input parameters used, the fraction of organic carbon (f_{oc}) used for the SSL modeling effort was slightly different than that used for the HWIR modeling effort. The f_{oc} used for the SSL effort was equal to 0.002 g/g, which better reflected average subsurface conditions at Superfund sites. This value is approximately equal to the high value of organic carbon used in the HWIR modeling effort.

Table 44. Summary of Geochemical Parameters Used in SSL MINTEQ Modeling Effort

Value	pH	Iron oxide content (weight percent)
Low	4.9	0.01
Medium	6.8	0.31
High	8.0	1.11

Source: U.S. EPA (1992a)

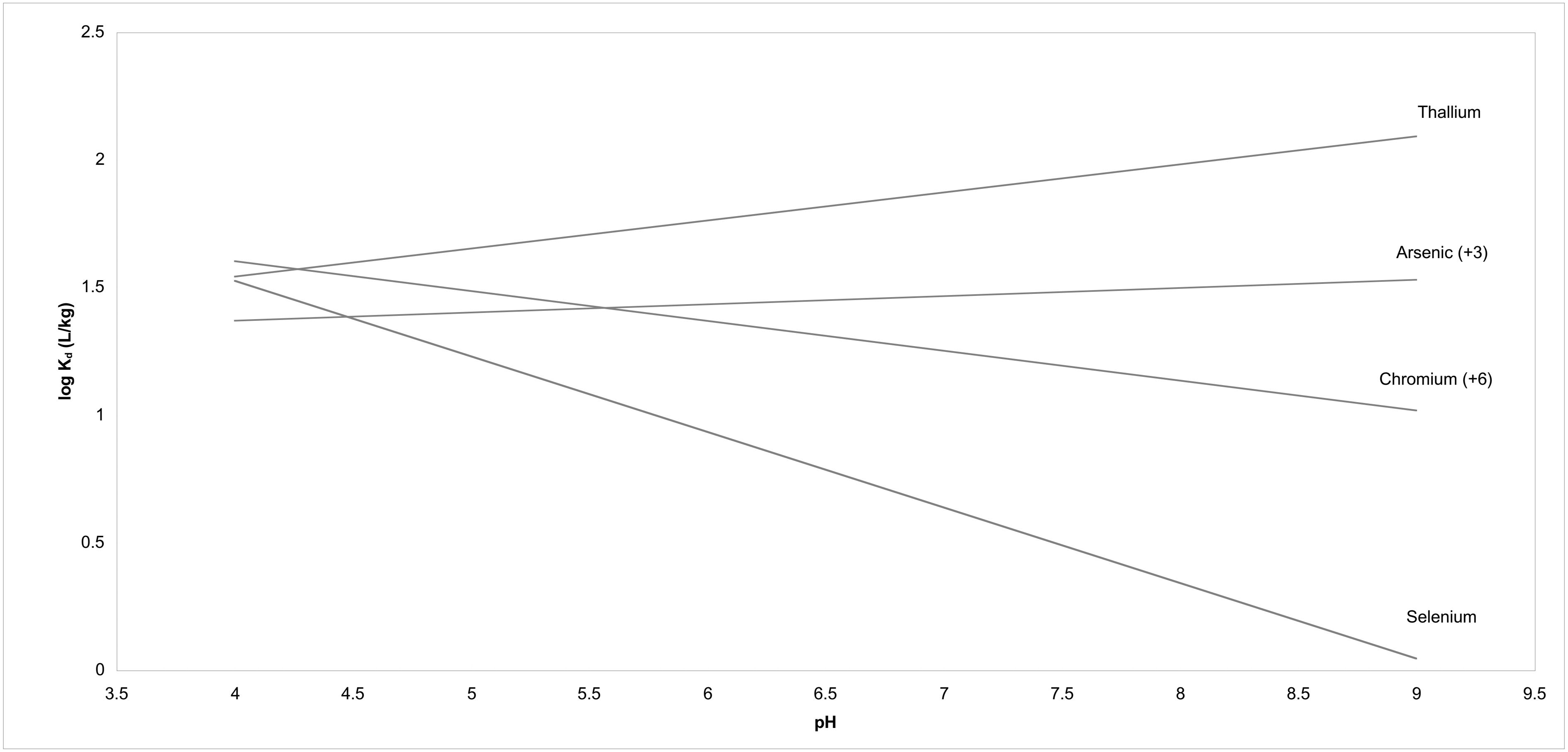


Figure 10. Empirical pH-dependent adsorption relationship: arsenic (+3), chromium

Table 45. Background Pore-Water Chemistry Assumed for SSL MINTEQ Modeling Effort[a]

Parameter	Concentration (mg/L)
Aluminum	0.2
Bromine	0.3
Calcium	48
Carbonate	187
Chlorine	15
Iron (+3)	0.2
Magnesium	14
Manganese (+2)	0.04
Nitrate	1
Phosphate	0.09
Potassium	2.9[b]
Sodium	22
Sulfate	25

[a] Median values from STORET database as reported in U.S. EPA (1992a).

[b] Median values from STORET database; personal communication from J. Allison, Allison Geosciences.

5.4.3. Assumptions and Limitations. The SSL MINTEQ modeling effort incorporates several basic simplifying assumptions. In addition, the applicability and accuracy of the model results are subject to limitations. Some of the more significant assumptions and limitations are described below.

- **The system is assumed to be at equilibrium.** This assumption is inherent in geochemical aqueous speciation models because the fundamental equations of mass action and mass balance are equilibrium based. Therefore, any possible influence of adsorption (or desorption) rate limits is not considered.

  This assumption is **conservative**. Because the model is being used to simulate metal desorption from the solid substrate, if equilibrium conditions are not met, the desorption reaction will be incomplete and the metal concentration in pore water will be less than predicted by the model.

- **Redox potential is not considered.** The redox potential of the system is not considered due to the difficulty in obtaining reliable field measurements of oxidation reduction potential (Eh), which are needed to determine a realistic frequency distribution of this parameter. Furthermore, the geochemistry of redox-sensitive species is poorly understood. Reactions involving redox species are often biologically mediated and the concentrations of redox species are not as likely to reflect thermodynamic equilibrium as other inorganic constituents.

  To provide a **conservative** estimate of metal mobility, all environmentally viable oxidation states are modeled separately for the redox-sensitive metals; the most conservative was selected for defining SSL metal K_d values. The redox-sensitive constituents that make up the background chemistry are represented only by the oxidation state that most enhances metal mobility (U.S. EPA, 1992a).

- **Potential sorbent surfaces are limited.** Only metal adsorption to FeOx and solid organic matter is considered in the system. It is recognized that numerous other natural sorbents exist (e.g., clay and carbonate minerals); however, thermodynamic databases describing metal adsorption to these surfaces are not available and the potential for adsorption to such surfaces is not considered. This assumption is **conservative** and will underpredict sorption for soils with significant amounts of such sorption sites.

- **The available thermodynamic database is limiting.** As metal behavior increases in complexity, thermodynamic data become more rare. The lack of complete thermodynamic data requires simplification to the defined system. This simplification may be **conservative** or **nonconservative** in terms of metal mobility.

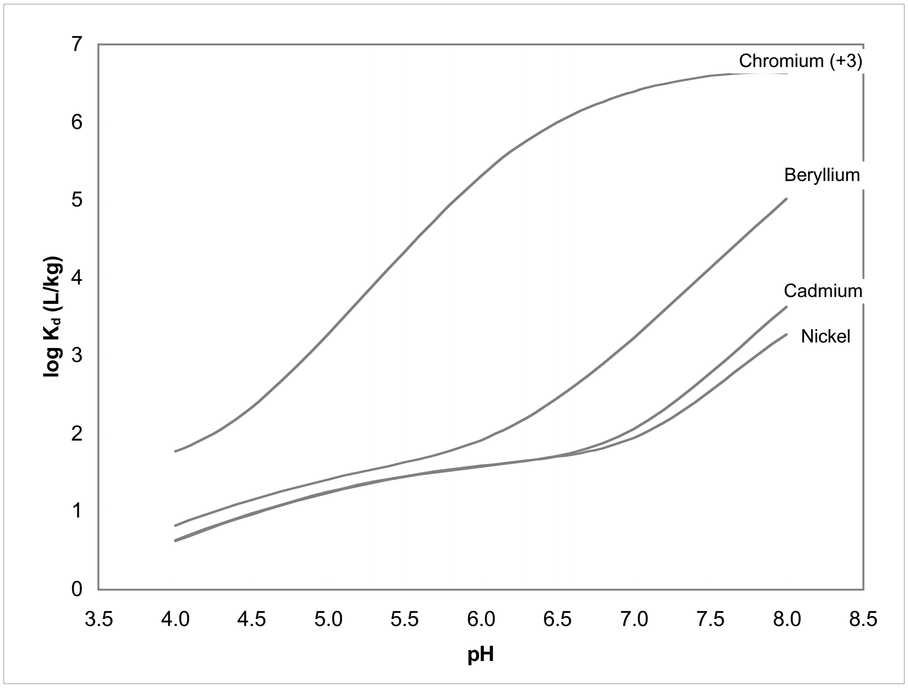
- **Metal competition is not considered.** Model simulations were performed for systems comprised of only one metal (i.e., the potential for competition between multiple metals for available sorbent surface sites was not considered). Generally, the competition of multiple metals for available sorption sites results in higher dissolved metal concentrations than would exist in the absence of competition. Consequently, this assumption is **nonconservative** but is significant only at metal concentrations much higher than the SSLs.

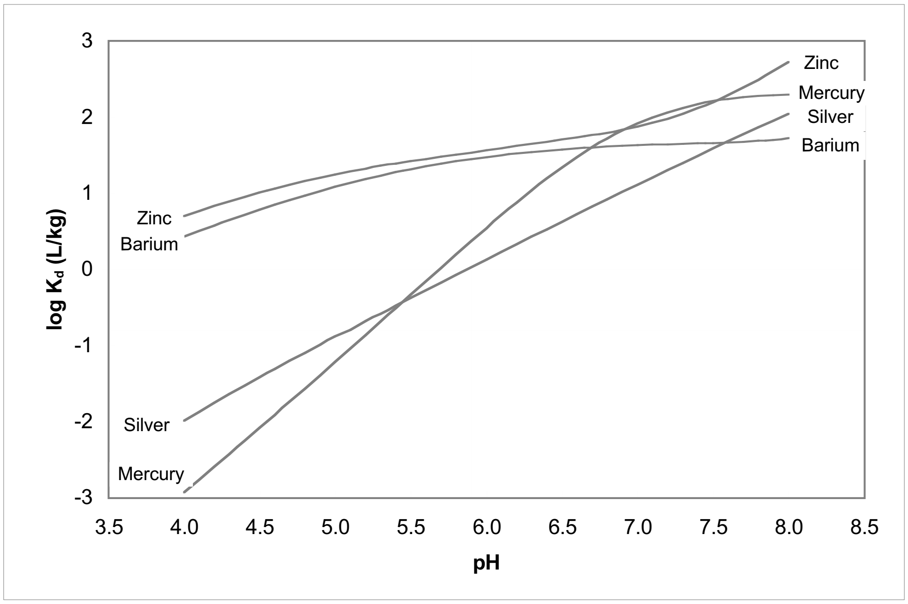
Other assumptions and limitations associated with this modeling effort are discussed in RTI (1994).

5.4.4 Results and Discussion. MINTEQ model results indicate that metal mobility is most affected by changes in pH. Based on this observation and because iron oxide content is not routinely measured in site characterization efforts, pH-dependent K_ds for metals were developed for SSL application by fixing iron oxide at its medium value and fraction organic carbon at 0.002. For arsenic (+3), chromium (+6), selenium, and thallium, the empirical pH-dependent K_ds were used.

Table 46 shows the SSL K_d values at high, medium, and low subsurface pH conditions. Figure 11 plots MINTEQ-derived metal K_d values over this pH range. Figure 10 shows the same for the empirically derived metal K_ds. These results are discussed below by metal and compared with measured values. See RTI (1994) for more information. pH-dependent values are not available for antimony, cyanide, and vanadium. The estimated K_d values shown in Table 46 for antimony and vanadium are reported by Baes et al. (1984) and the K_d value for cyanide is obtained from SCDM.

Arsenic. K_d values developed using the empirical equation for arsenic (+3) range from 25 to 31 L/kg for pH values of 4.9 to 8.0, respectively. These values correlate fairly well with the range of measured values reported by Battelle (1989)—5.86 to 19.4 L/kg. They are slightly above the range reported by Baes and Sharp (1983) for arsenic (+3) (1.0-8.3). The estimated K_d values for arsenic (+3) do not correlate well with the value of 200 L/kg presented by Baes et al. (1984). Oxidation state is not specified in Baes et al. (1984), and the difference between the empirical-derived K_d values presented here and the value presented by Baes et al. (1984) may reflect differences in oxidation states (arsenic (+3) is the most mobile species).





Note: Conditions depicted are medium iron oxide content (0.31 wt %) and organic matter of 0.2 wt %.

Figure 11. Metal Kd as a function of pH.

Table 46. Estimated Inorganic K_d Values for SSL Application

Metal	Estimated K_d (L/kg) **pH = 4.9**	 **pH = 6.8**	 **pH = 8.0**
Antimony[a]		4.5E+01	
Arsenic (+3)[b]	2.5E+01	2.9E+01	3.1E+01
Barium	1.1E+01	4.1E+01	5.2E+01
Beryllium	2.3E+01	7.9E+02	1.0E+05
Cadmium	1.5E+01	7.5E+01	4.3E+03
Chromium (+3)	1.2E+03	1.8E+06	4.3E+06
Chromium (+6)[b]	3.1E+01	1.9E+01	1.4E+01
Cyanide[c]		9.9E+00	
Mercury (+2)	4.0E-02	5.2E+01	2.0E+02
Nickel	1.6E+01	6.5E+01	1.9E+03
Selenium[b]	1.8E+01	5.0E+00	2.2E+00
Silver	1.0E-01	8.3E+00	1.1E+02
Thallium[b]	4.4E+01	7.1E+01	9.6E+01
Vanadium[a]		1.0E+03	
Zinc	1.6E+01	6.2E+01	5.3E+02

[a] Geometric mean measured value from Baes et al., 1984 (pH-dependent values not available).
[b] Determined using an empirical pH-dependent relationship (Figure 10).
[c] SCDM = Superfund Chemical Data Matrix (pH-dependent values not available).

Barium. For ground water pH conditions, MINTEQ-estimated K_d values for barium range from 11 to 52 L/kg. This range correlates well with the value of 60 L/kg reported by Baes et al. (1984). Battelle (1989) reports a range in K_d values from 530 to 16,000 L/kg for a pH range of 5 to 9. The model-predicted K_d values for barium are several orders of magnitude less than the measured values, possibly due to the lower sorptive potential of iron oxide, used as the modeled sorbent, relative to clay, a sorbent present in the experimental systems reported by Battelle (1989).

Beryllium. The K_d values estimated for beryllium range from 23 to 100,000 L/kg for the conditions studied. AECL (1990) reports medians of observed values for K_d ranging from 250 L/kg for sand to 3,000 L/kg for organic matter. Baes et al. (1984) report a value of 650 L/kg. Battelle (1989) reports a range of K_d values from 70 L/kg for sand to 8,000 L/kg for clay. MINTEQ results for medium ground water pH (i.e., a value of 6.8) yields a K_d value of 790 L/kg. Hence, there is reasonable agreement between the MINTEQ-predicted K_d values and values reported in the literature.

Cadmium. For the three pH conditions, MINTEQ K_d values for cadmium range from 15 to 4,300 L/kg, with a value of 75 at a pH of 6.8. The range in experimentally determined K_d values for cadmium is as follows: 1.26 to 26.8 L/kg (Baes et al., 1983), 32 to 50 L/kg (Coughtrey et al., 1985), 14.9 to 567 L/kg (Battelle, 1989), and 2.7 to 17,000 L/kg (AECL, 1990). Thus the MINTEQ estimates are generally within the range of measured values.

Chromium (+3). MINTEQ-estimated K_d values for chromium (+3) range from 1,200 to 4,300,000 L/kg. Battelle (1989) reports a range of K_d values of 168 to 3,600 L/kg, orders of magnitude lower than the MINTEQ values. This difference may reflect the measurements of mixed systems comprised of both chromium (+3) and (+6). The incorporation of chromium (+6) would tend to lower the K_d. Because the model-predicted values may overpredict sorption, the user should exercise care in the use of these values. Values for chromium (+6) should be used where speciation is mixed or uncertain.

Chromium (+6). Chromium (+6) K_d values estimated using the empirical pH-dependent adsorption relationship range from 31 to 14 L/kg for pH values of 4.9 to 8.0. Battelle (1989) reports a range of 16.8 to 360 L/kg for chromium (+6) and Baes and Sharp (1983) report a range of 1.2 to 1,800. The predicted chromium (+6) K_d values thus generally agree with the lower end of the range of measured values and the average measured values (37) reported by Baes and Sharp (1983). These values represent conservative estimates of mobility the more toxic of the chromium species.

Mercury (+2). MINTEQ-estimated K_d values for mercury (+2) range from 0.04 to 200 L/kg. These model-predicted estimates are less than the measured range of 322 to 5,280 L/kg reported by Battelle (1989). This difference may reflect the limited thermodynamic database with respect to mercury and/or that only the divalent oxidation state is considered in the simulation. Allison (1993) reviewed the model results in comparison to the measured values reported by Battelle (1989) and found reasonable agreement between the two sets of data, given the uncertainty associated with laboratory measurements and model precision.

Nickel. MINTEQ-estimated K_d values for nickel range from 16 to 1,900 L/kg. These values agree well with measured values of approximately 20 L/kg (mean) and 12.2 to 650 L/kg, reported by Coughtrey et al. (1985) and Battelle (1989), respectively. These values also agree well with the value of 150 L/kg reported by Baes et al. (1984). However, the predicted values are at the low end of the range reported by the AECL (1990)—60 to 4,700 L/kg.

Selenium. Empirically derived K_d values for selenium range from 2.2 to 18 L/kg for pH values of 8.0 to 4.9. The range in experimentally determined K_d values for selenium is as follows: less than 9 L/kg (Coughtrey et al., 1985), 5.9 to 14.9 L/kg (Battelle, 1989), and 150 to 1,800 L/kg (AECL, 1990). Baes et al. (1984) reported a value of 300 L/kg. Although they are significantly below the values presented by the AECL (1990) and Baes et al. (1984), the MINTEQ-predicted K_d values correlate well with the values reported by Coughtrey et al. (1985) and Battelle (1989).

Silver. The K_d values estimated for silver range from 0.10 to 110 L/kg for the conditions studied. The range in experimentally determined K_d values for silver is as follows: 2.7 to 33,000 L/kg (AECL, 1990), 10 to 1,000 L/kg (Baes et al., 1984), 50 L/kg (Coughtrey et al., 1985), and 0.4 to 40 L/kg (Battelle, 1989). The model-predicted K_d values agree well with the values reported by Coughtrey et al. (1985) and Battelle (1989) but are at the lower end of the ranges reported by AECL (1990) and Baes et al. (1984).

Thallium. Empirically derived K_d values for thallium range from 44 to 96 L/kg for pH values of 4.9 to 8.0. Generally, these values are about an order of magnitude greater than those reported by Battelle (1989)—0.0 to 0.8 L/kg - but are well below the value predicted by Baes et al. (1984).

Zinc. MINTEQ-estimated K_d values for zinc range from 16 to 530 L/kg. These estimated K_d values are within the range of measured K_d values reported by the AECL (1990) (0.1 to 100,000 L/kg) and Baes et al. (1984) (0.1 to 8,000 L/kg). Coughtrey et al. (1985) reported a K_d value for zinc of greater than or equal to 20 L/kg.

5.4.5 Analysis of Peer-Review Comments. A peer review was conducted of the model assumptions and inputs used to estimate K_d values for SSL application. This review identified several issues of concern, including:

- The charge balance exceeds an acceptable margin of difference (5 percent) in most of the simulations. A variance in excess of 5 percent may indicate that the model problem is not correctly chemically poised and therefore the results may not be chemically meaningful.
- The model should not allow sulfate to adsorb to the iron oxide. Sulfate is a weakly outer-sphere adsorbing species and, by including the adsorption reaction, sulfate is removed from the aqueous phase at pH values less than 7 and is prevented from participating in precipitation reaction at these pH values.
- Modeled K_d values for barium and zinc could not be reproduced for all studied conditions.

A technical analysis of these concerns indicated that, although these comments were based on true observations about the model results, these factors do not compromise the validity of the MINTEQ results in this application. This technical analysis is provided in Appendix M.

Part 6: REFERENCES

Abdul, A.S., T.L. Gibson, and D.N. Rai. 1987. Statistical correlations for predicting the partition coefficient for nonpolar organic contaminants between aquifer carbon and water. *Hazardous Waste and Hazardous Materials* 4(3):211-223.

AECL (Atomic Energy of Canada Limited). 1990. *A Critical Compilation and Review of Default Soil Solid/Liquid Partition Coefficients, K_d, for Use in Environmental Assessments,* by D.H. Thibault, M.I. Sheppard, and P.A. Smith, Whiteshell Nuclear Research Establishment, Pinawa, Manitoba.

Aller, L., T. Bennett, J.H. Lehr, R.J. Petty, and G. Hackett. 1987. *DRASTIC: A Standardized System for Evaluating Ground Water Pollution Potential Using Hydrogeologic Settings.* EPA-600/2-87-035. Prepared for U.S. EPA Office of Research and Development, Ada, OK. National Water Well Association, Dublin, OH.

Allison, J. 1993. *Review and Evaluation of the MINTEQA2 K_d Results for Mercury in the Finite Source Methodology.* Prepared by Allison Geoscience Consultants, Inc., for the U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

ASTM (American Society for Testing and Materials). 1994. Risk-Based Corrective Action Guidance. Philadelphia, PA. (Draft).

Baes, C.F. (III), and R.D. Sharp. 1983. A proposal for estimation of soil leaching and leaching constants for use in assessment models. *J. Environ. Qual.* 12(1):17-28.

Baes, C.F. (III), R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. *A Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides through Agriculture*. Oak Ridge National Laboratory Report ORNL-5786. ORNL, Oak Ridge, TN.

Battelle Memorial Institute. 1989. *Chemical Data Bases for the Multimedia Environmental Pollutant Assessment System (MEPAS): Version 1.* Prepared for the U.S. Department of Energy under Contract DE-AC06-76RKI 1830, by Pacific Northwest Laboratory, operated by Battelle Memorial Institute.

Boyd, S.A. 1982. Adsorption of substituted phenols by soil. *Soil Science,* 134(5):337-343.

Brady, N.C. 1990. *The Nature and Properties of Soils.* Macmillan Publishing Company, New York, NY.

Calabrese, E.J., H. Pastides, R. Barnes, et al. 1989. How much soil do young children ingest: an epidemiologic study. In: *Petroleum Contaminated Soils*, Vol. 2. E.J. Calabrese and P.T. Kostecki, eds. pp. 363-417. Chelsea, MI, Lewis Publishers.

Carsel, R.F., and R.S. Parrish. 1988. Developing joint probability distributions of soil water retention characteristics. *Water Resources Research*, 24(5):755-769.

Carsel, R.F., R.S. Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. Characterizing the uncertainty of pesticide leaching in agricultural soils. *J. of Contam. Hyd.* 2:111-124.

Chen, L. 1995. Testing the mean of skewed distributions. *Journal of the American Statistical Association* 90(430):767-772.

Coughtry, P.J., D. Jackson, and M.C. Thorne. 1985. *Radionuclide Distribution and Transporting Terrestrial and Aquatic Ecosystems: A Compendium of Data.* A.A. Balkem, Netherlands, Vol. 6.

Cowherd, C., G. Muleski, P. Engelhart, and D. Gillette. 1985. *Rapid Assessment of Exposure to Particulate Emissions from Surface Contamination*. EPA/600/8-85/002. NTIS PB85-192219. Office of Health and Environmental Assessment, U.S. Environmental Protection Agency, Washington, DC.

Criscenti, L.J., S.B. Christian, E.Z. Hosseinipour, and V.M. Gorokhovski. 1994. *Evaluation of Unsaturated Zone/Vadose Zone Models for Superfund Sites. Draft Report*. Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Athens, GA.

Curtis, G. P., P. V. Roberts, and M. Reinhard. 1986. A natural gradient experiment on solute transport in a sand aquifer. *Water Resources Research* 22(13):2059-2067.

Davis, S., P. Waller, R. Buschom, J. Ballou, and P. White. 1990. Quantitative estimates of soil ingestion in normal children between the ages of 2 and 7 years: population-based estimates using Al, Si, and Ti as soil tracer elements. *Archives of Environmental Health* 45:112-122.

Di Toro, D.M. 1985. A particle interaction model of reversible organic chemical sorption. *Chemosphere* 14(10):1503-1538.

Dragun, J. 1988. *The Soil Chemistry of Hazardous Materials*. Hazardous Materials Control Research Institute, Silver Spring, MD.

EQ (Environmental Quality Management). 1992. *Limited Validation of the Hwang and Falco Model for Emissions of Soil-Incorporated Volatile Organic Compounds.* Contract No. 68-D8-0111. Prepared for Office of Emergency and Remedial Response, U.S. Environmental Protection Agency, Washington, DC.

EQ (Environmental Quality Management). 1993. *Evaluation of the Dispersion Equations in the Risk Assessment Guidance for Superfund (RAGS): Volume I—Human Health Evaluation Manual (Part B, Development of Preliminary Remediation Goals).* Contract No. 68-02-D120. Prepared for Office of Emergency and Remedial Response, U.S. Environmental Protection Agency, Washington, DC.

EQ (Environmental Quality Management). 1994. Revisions to VF and PEF Equations. Memorandum #5099-3. Prepared for Office of Emergency and Remedial Response, U.S. Environmental Protection Agency, Washington, DC.

EQ (Environmental Quality Management) and Pechan (E. H. Pechan and Associates). 1994. *A Comparison of Soil Volatilization Models in Support of Superfund Soil Screening Level Development*. Contract No. 68-D3-0035. Prepared for Office of Emergency and Remedial Response, U.S. Environmental Protection Agency, Washington, DC.

EQ (Environmental Quality Management). 1995. *Limited Validation of the Jury Infinite Source and Jury Reduced Solution Finite Source Models for Emissions of Soil-Incorporated Volatile Organic Compounds*. Prepared for Office of Solid Waste and Emergency Response, U.S. Environmental Protection Agency, Washington, DC.

Farmer, W. J., and J. Letey. 1974. *Volatilization Losses of Pesticides from Soils*. EPA-660/2-74/054. Office of Research and Development, U.S. Environmental Protection Agency, Washington, DC.

Feenstra, S., D.M. MacKay, and J.A. Cherry. 1991. A method for assessing residual NAPL based on organic chemical concentrations in soil samples. *Ground Water Monitoring Rev.* 11(2):128-136.

Gee, G.W., and J.W. Bauder. 1986. Particle size analysis. *In:* A. Klute (ed.), *Methods of Soil Analysis. Part 1. Physical and Mineralogical Methods. 2nd Edition,* 9(1):383-411, American Society of Agronomy, Madison, WI.

Gelhar, L.W., and C.J. Axness. 1981. *Stochastic Analysis of Macro-Dispersion in Three-Dimensionally Heterogeneous Aquifers.* Report No. H-8. Hydraulic Research Program. New Mexico Institute of Mining and Technology, Socorro, NM.

Gilbert, Richard O. 1987. *Statistical Methods for Environmental Pollution Monitoring.* New York: Van Nostrand Reinhold.

Hardin, J.W., and R.O. Gilbert. 1993. *Comparing Statistical Tests for Detecting Soil Contamination Greater than Background.* Pacific Northwest Laboratory (PNL-8989), Richard, WA.

Heath, R.C. 1984. *Ground-Water Regions of the United States.* USGS Water Supply Paper 2242. U.S. Geological Survey, Reston, VA.

Howard, P. H. 1989. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Vol. I. Large Production and Priority Pollutants.* Lewis Publishers, Chelsea, MI.

Hwang, S. T., and J. W. Falco. 1986. *Estimation of Multimedia Exposure Related to Hazardous Waste Facilities*. Y. Cohen, Ed. Plenum Publishing.

Johnson, N.L. 1978. Modified t tests and confidence intervals for asymmetrical populations. *Journal of the American Statistical Association* 73(363):536-544.

Johnson, P.C. and R.A. Ettinger. 1991. Heuristic model for predicting the intrusion rate of contaminant vapors into buildings. *Environmental Science and Technology* 25(8):1445-1452.

Jury, W.A., W.F. Spencer, and W.J. Farmer. 1983. Behavior assessment model for trace organics in soil: I. Model description. *J. Environ. Qual.* 12(4):558-564.

Jury, W.A., W.J. Farmer, and W.F. Spencer. 1984. Behavior assessment model for trace organics in soil: II. Chemical classification and parameter sensitivity. *J. Environ. Qual.* 13(4):567-572.

Jury, W.A., D. Russo, G. Streile, and H.E. Abd. 1990. Evaluation of volatilization by organic chemicals residing below the soil surface. *Water Resources Research* 26(1):13-20.

Karickhoff, S.W. 1984. Organic pollutant sorption in aquatic systems. *J. Hydraul. Eng*. 110(6):707-735.

Kollig, H.P. 1993. *Environmental Fate Constants for Organic Chemicals under Consideration for EPA's Hazardous Waste Identification Projects.* Office of Research and Development, U.S. Environmental Protection Agency, Washington, DC.

Kukowski, H. 1989. *Adsorption and Desorption of Ionizable Organic Chemicals by Soils.* Ph.D. Dissertation, University of Kiel.

Land, C.E. 1971. Confidence intervals for linear functions of the normal mean and variance. *Annals of Mathematical Statistics* 42:1187-1205.

Land, C.E. 1975. Tables of confidence limits for linear functions of the normal mean and variance. *Selected Tables in Mathematical Statistics*, 3:385-419. American Mathematical Society, Providence, RI.

Lee, L. S., P. S. C. Rao, P. Nkedi-Kizza, and J. J. Delfino. 1990. Influence of solvent and sorbent characteristics on distribution of pentachlorophenol in octanol-water and soil-water systems. *Environ. Sci. Tech*. 24:654-661.

Lee, L. S., P. S. C. Rao, and M. L. Brusseau. 1991. Nonequilibrium sorption and transport of neutral and ionized compounds. *Environ. Sci. Tech*. 25:722-729.

Lyman, W. J., W. F. Reehl, and D. H. Rosenblatt. 1982. *Handbook of Chemical Property Estimation Methods*. McGraw-Hill, New York.

Marshall, J. 1971. Drag measurements in roughness arrays of varying density and distribution. *Agricultural Meteorology*, 8:269-292.

McCarty, P.L., M. Reinhard, and B.E. Rittmann. 1981. Trace organics in ground water. *Environ. Sci. Technol.* 15:40-51.

McLean, E.O. 1982. Soil pH and lime requirement. *In:* A.L. Page (ed.), *Methods of Soil Analysis. Part 2. Chemical and Microbiological Properties. 2nd Edition,* 9(2):199-224, American Society of Agronomy, Madison, WI.

Meylan, W., P.H. Howard, and R.S. Boethling. 1992. Molecular topology/fragment contribution method for predicting soil sorption coefficients. *Environ. Sci. Technol.* 26(8):1560-1567.

Miller, R.G. 1991. *Simultaneous Statistical Inference*. 2nd edition. Springer-Verlag, New York.

Millington, R. J., and J. M. Quirk. 1961. Permeability of porous soils. *Trans. Faraday Soc.* 57:1200-1207.

Nelson, D.W., and L.E. Sommers. 1982. Total carbon, organic carbon, and organic matter. *In:* A.L. Page (ed.), *Methods of Soil Analysis. Part 2. Chemical and Microbiological Properties. 2nd Edition,* 9(2):539-579, American Society of Agronomy, Madison, WI.

Newell, C.J., L.P. Hopkins, and P.B. Bedient. 1989. *Hydrogeologic Database for Ground Water Modeling.* API Publication No. 4476. American Petroleum Institute, Washington, DC.

Newell, C.J., L.P. Hopkins, and P.B. Bedient. 1990. A hydrogeologic database for ground water-modeling. *Ground Water,* 28(5):703-714.

Nofziger, D.L., J. Chen, and C.T. Haan. 1994. *Evaluation of Unsaturated/Vadose Zone Models for Superfund Sites.* EPA/600/R-93/184. Office of Research and Development, U.S. Environmental Protection Agency, Robert S. Kerr Environmental Research Laboratory, Ada, OK.

Piwoni, M. D., and P. Banerjee. 1989. Sorption of volatile organic solvents from aqueous solution onto subsurface solids. *J. Contam. Hydrol*. 4(2):163-179.

Radian. 1989. *Short-term Fate and Persistence of Motor Fuels in Soils.* Report to the American Petroleum Institute, Washington, DC.

RTI (Research Triangle Institute). 1994. *Chemical Properties for Soil Screening Levels. Draft Report*. Prepared for Office of Emergency and Remedial Response, U.S. Environmental Protection Agency, Washington, DC.

Salhotra, A.M., P. Mineart, S. Sharp-Hansen, and T. Allison. 1990. *Multimedia Exposure Assessment Model (MULTIMED) for Evaluating the Land Disposal of Wastes—Model Theory.* Environmental Research Laboratory, U.S. Environmental Protection Agency, Athens, GA.

Schellenberg K., C. Leuenberger, and R.P. Schwarzenbach. 1984. Sorption of chlorinated phenols by natural sediments and aquifer materials. *Environ. Sci. Technol.* 18(9):652-657.

Schwarzenbach, R. P., and J. C. Westall. 1981. Transport of non-polar organic compounds from surface water to ground water. *Environ. Sci. Tech*. 15(11):1360-1367.

Shan, C., and D.B. Stephens. 1995. An analytical solution for vertical transport of volatile chemicals in the vadose zone. *Journal of Contaminant Hydrology* 18:259-277.

Sharp-Hansen, S., C. Travers, P. Hummel, and T. Allison. 1990. *A Subtitle D Landfill Application Manual for the Multimedia Exposure Assessment Model (MULTIMED).* EPA Contract No. 68-03-3513. Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Athens, GA.

Shimizu, Y., N. Takei, S. Yamakazi, and Y. Terashima. 1993. *Sorption of Organic Pollutants onto Natural Solids: Ionizable Organics in a Saturated System and Volatile Organics in an Unsaturated System.* Selected Papers on Environmental Hydrogeology, 29th International Geologic Congress, Kyoto, Japan, Volume 4, August 24-September 3, 1993.

U.S. EPA (Environmental Protection Agency). 1980. *Land Disposal of Hexachlorobenzene Wastes Controlling Vapor Movement in Soil.* EPA-600/2-80-119. Office of Research and Development, Cincinnati, OH. NTIS PB80-216575.

U.S. EPA (Environmental Protection Agency). 1988. *Superfund Exposure Assessment Manual.* OSWER Directive 9285.5-1. EPA/540/1-88/001. Office of Emergency and Remedial Response, Washington, DC. NTIS PB89-135859

U.S. EPA (Environmental Protection Agency). 1989a. *Methods for Evaluating the Attainment of Soil Cleanup Standards. Volume 1: Soils and Solid Media*. EPA 230/02-89-042. Statistical Policy Branch, Office of Policy, Planning and Evaluation, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1989b. *Risk Assessment Guidance for Superfund, Volume 1: Human Health Evaluation Manual, Part A, Interim Final.* EPA/540/1-89/002. Publication 9285.7-01A. Office of Emergency and Remedial Response, Washington, DC. NTIS PB90-155581/CCE.

U.S. EPA (Environmental Protection Agency). 1990. *Guidance on Remedial Actions for Superfund Sites with PCB Contamination*. Office of Solid Waste and Emergency Response, Washington, DC. NTIS PB91-1921206CDH.

U.S. EPA (Environmental Protection Agency). 1990. *Sampler's Guide to the Contract Laboratory Program*. Office of Emergency and Remedial Response, Washington, DC. NTIS-PB91-921330CDH.

U.S. EPA (Environmental Protection Agency). 1991a. *Human Health Evaluation Manual, Supplemental Guidance: Standard Default Exposure Factors.* Publication 9285.6-03. Office of Emergency and Remedial Response, Washington, DC. NTIS PB91-921314.

U.S. EPA (Environmental Protection Agency). 1991b. *Risk Assessment Guidance for Superfund, Volume I: Human Health Evaluation Manual (Part B, Development of Risk-Based Preliminary Remediation Goals). Interim.* Publication 9285.7-01B. Office of Emergency and Remedial Response, Washington, DC. NTIS PB92-963333.

U.S. EPA (Environmental Protection Agency). 1991c. *Role of the Baseline Risk Assessment in Superfund Remedy Selection Decisions.* Publication 9355.0-30. Office of Emergency and Remedial Response, Washington, DC. NTIS PB91-921359/CCE.

U.S. EPA (Environmental Protection Agency). 1991d. *User's Guide to the Contract Laboratory Program*. Office of Emergency and Remedial Response, Washington, DC. NTIS-PB91-921278CDH.

U.S. EPA (Environmental Protection Agency). 1992a. *Background Document for Finite Source Methodology for Wastes Containing Metals*. HWEP-S0040. Office of Solid Waste, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1992b. *Dermal Exposure Assessment: Principles and Applications*. Interim Report. EPA/600/8-91/011B. Office of Research and Development, Cincinnati, OH.

U.S. EPA (Environmental Protection Agency). 1992c. *Estimating the Potential for Occurrence of DNAPL at Superfund Sites.* Pub. 9355.4-07FS. Office of Solid Waste and Emergency Response, Washington, DC. R.S. Kerr Environmental Research Laboratory, Ada, OK. NTIS PB92-963358.

U.S. EPA (Environmental Protection Agency). 1992d. *Technical Support Document for Land Application of Sewage Sludge. Volumes 1 and 2.* EPA 822/R-93-001A,B. Office of Water, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1992e. *Handbook of RCRA Ground-Water Monitoring Constituents: Chemical and Physical Properties*. EPA/530-R-92-022. Office of Solid Waste, Washington, DC. NTIS PB92-233287.

U.S. EPA. (Environmental Protection Agency). 1992f. *Preparation of Soil Sampling Protocols: Sampling Techniques and Strategies.* Office of Research and Development, Washington, DC. EPA/600/R-92/128.

U.S. EPA (Environmental Protection Agency). 1993a. *Background Document for EPA's Composite Model for Leachate Migration with Transformation Products, EPACMTP*. Office of Solid Waste, Washington, DC. July.

U.S. EPA (Environmental Protection Agency). 1993b. *Data Quality Objectives for Superfund: Interim Final Guidance*. EPA 540-R-93-071. Publication 9255.9-01. Office of Emergency and Remedial Response, Washington, DC. NTIS PB94-963203.

U.S. EPA (Environmental Protection Agency). 1993c. *Provisional Guidance for the Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons.* Office of Health Effects Assessment, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1993d. *Quality Assurance for Superfund Environmental Data Collection Activities.* Quick Reference Fact Sheet. Office of Emergency and Remedial Response, Washington, DC. NTIS PB93-963273.

U.S. EPA (Environmental Protection Agency). 1993e. Science Advisory Board Review of the Office of Solid Waste and Emergency Response draft *Risk Assessment Guidance for Superfund (*RAGS*), Human Health Evaluation Manual (*HHEM*).* EPA-SAB-EHC-93-007. Science Advisory Board, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1993f. *The Urban Soil Lead Abatement Demonstration Project. Vol I: Integrated Report Review Draft.* EPA-600/AP93001/A. NTIS PB93-222-651.

U.S. EPA (Environmental Protection Agency). 1994. *Revised Interim Soil Lead Guidance for CERCLA Sites and RCRA Corrective Action Facilities*. Office of Solid Waste and Emergency Response, Washington, DC. Directive 9355.4-12.

U.S. EPA (Environmental Protection Agency). 1994a. *Framework for Assessing Ground Water Modeling Applications.* EPA-500-B-94-004. Resource Management and Information Staff, Office of Solid Waste and Emergency Response, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1994b. *Ground Water Modeling Compendium, Second Edition.* EPA-500-B-94-003. Resource Management and Information Staff, Office of Solid Waste and Emergency Response, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1994c. *Guidance for the Data Quality Objectives Process*. EPA QA/G-4. Quality Assurance Management Staff, Office of Research and Development, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1994d. *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry.* EPA/600/8-90/066F. Office of Research and Development, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1994e. *Methods for Evaluating the Attainment of Cleanup Standards—Volume 3: Reference-Based Standards for Soils and Solid Media.* EPA 230-R-94-004. Environmental Statistics and Information Division, Office of Policy, Planning, and Evaluation, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1994f. Risk Assessment Issue Paper for: Derivation of a Provisional RfD for *1,1-Dichloroethane* (75-34-3). Environmental Criteria Assessment Office, Cincinnati, OH.

U.S. EPA (Environmental Protection Agency). 1994g. Risk Assessment Issue Paper for: Provisional Oral RfD for *Naphthalene* (91-20-3). Environmental Criteria Assessment Office, Cincinnati, OH.

U.S. EPA (Environmental Protection Agency). 1994h. *Soil Screening Level Guidance.* Quick Reference Fact Sheet. Draft. Office of Emergency and Remedial Response, Washington, DC. NTIS PB93-963508.

U.S. EPA (Environmental Protection Agency). 1994i. *Technical Background Document for Soil Screening Guidance*. Draft. EPA/540/R-94/106. Office of Emergency and Remedial Response, Washington, DC. NTIS PB95-963532.

U.S. EPA (Environmental Protection Agency). 1995a. *Drinking Water Regulations and Health Advisories.* Office of Water, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1995b. Integrated Risk Information System (IRIS). Cincinnati, OH. December.

U.S. EPA (Environmental Protection Agency). 1995d. *Health Effects Assessment Summary Tables: FY-1995 Annual*. EPA540/R-95-036. Office of Research and Development. Office of Emergency and Remedial Response, Washington, DC. NTIS PB95-921199.

U.S. EPA (Environmental Protection Agency). 1996. *Soil Screening Guidance: User's Guide*. EPA/540/R-96/018. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96.9634501

Van der Heijde, P.M. 1994. *Identification and Compilation of Unsaturated/Vadose Zone Models.* EPA/600/R-94/028. R.S. Kerr Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Ada, OK.

Van Wijnen, J.H., P. Clausing, and B. Brunekreef. 1990. Estimated soil ingestion by children. *Environmental Research*, 51:147-162.

Wester, R.C., H.I. Maibach, D.A.W. Bucks, L. Sedik, J. Melendres, C. Liao, and S. DiZio. 1990. Percutaneous absorption of [^{14}C]DDT and [^{14}C]Benzo[*a*]pyrene from soil. *Fund. App. Toxicol.* 15:510-516.

Wester, R.C., H.I. Maibach, and L. Sedik. 1993. Percutaneous absorption of pentachlorophenol from soil. *Fundamentals of Applied Toxicology,* 20.

Will, M.E. and G.W. Suter II. 1994. *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Terrestrial Plants: 1994 Revision.* ES/ER/TM-85/R1. Prepared for the U.S. Department of Energy by the Environmental Sciences Division of the Oak Ridge National Laboratory.

APPENDIX A

Generic SSLs

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Generic SSLs

Table A-1 provides generic SSLs for 110 chemicals. Generic SSLs are derived using default values in the standardized equations presented in Part 2 of this document. The default values (listed in Table A-2) are conservative and are likely to be protective for the majority of site conditions across the nation.

However, the generic SSLs are not necessarily protective of all known human exposure pathways, reasonable land uses, or ecological threats. Thus, before applying generic SSLs at a site, it is extremely important to compare the conceptual site model (see the *User's Guide)* with the assumptions behind the SSLs to ensure that the site conditions and exposure pathways match those used to develop generic SSLs (see Parts 1 and 2 and Table A-2). If this comparison indicates that the site is more complex than the SSL scenario, or that there are significant exposure pathways **not** accounted for by the SSLs, then generic SSLs are not sufficient for a full evaluation of the site. A more detailed site-specific approach will be necessary to evaluate the additional pathways or site conditions.

Generic SSLs are presented separately for major pathways of concern in both surface and subsurface soils. The first column to the right of the chemical name presents levels based on direct ingestion of soil and the second column presents levels based on inhalation. As discussed in the *User's Guide*, the fugitive dust pathway may be of concern for certain metals but does not appear to be of concern for organic compounds. Therefore, SSLs for the fugitive dust pathway are only presented for inorganic compounds. Except for mercury, no SSLs for the inhalation of volatiles pathway are provided for inorganic compounds because these chemicals are not volatile.

The user should note that several of the generic SSLs for the inhalation of volatiles pathway are determined by the soil saturation concentration (C_{sat}), which is used to address and screen the potential presence of nonaqueous phase liquids (NAPLs). As explained in Section 2.4.4, for compounds that are liquid at ambient soil temperature, concentrations above C_{sat} indicate a potential for free-phase liquid contamination to be present and the need for additional investigation.

The third column presents generic SSL values for the migration to ground water pathway developed using a default DAF (dilution-attenuation factor) of 20 to account for natural processes that reduce contaminant concentrations in the subsurface (see Section 2.5.6). SSLs in Table A-1 are rounded to two significant figures except for values less than 10, which are rounded to one significant figure. Note that the 20 DAF values in Table A-1 are not exactly 20 times the 1 DAF values because each SSL is calculated independently in both the 20 DAF and 1 DAF columns, with the final value presented according to the aforementioned rounding conventions.

The fourth column contains the generic SSLs for the migration to ground water pathway developed assuming no dilution or attenuation between the source and the receptor well (i.e., a DAF of 1). These values can be used at sites where little or no dilution or attenuation of soil leachate concentrations is expected at a site (e.g., sites with shallow water tables, fractured media, karst topography, or source size greater than 30 acres).

Generally, if an SSL is not exceeded for a pathway of concern, the user may eliminate the pathway or areas of the site from further investigation. If more than one exposure pathway is of concern, the lowest SSL should be used.

Table A-1. Generic SSLs [a]

Organics				Migration to ground water	
CAS No.	Compound	Ingestion (mg/kg)	Inhalation volatiles (mg/kg)	20 DAF (mg/kg)	1 DAF (mg/kg)
83-32-9	Acenaphthene	4,700 [b]	--- [c]	570 [b]	29 [b]
67-64-1	Acetone	7,800 [b]	1.0E+05 [d]	16 [b]	0.8 [b]
309-00-2	Aldrin	0.04 [e]	3 [e]	0.5 [e]	0.02 [e]
120-12-7	Anthracene	23,000 [b]	--- [c]	12,000 [b]	590 [b]
56-55-3	Benz(*a*)anthracene	0.9 [e]	--- [c]	2 [e]	0.08 [e,f]
71-43-2	Benzene	22 [e]	0.8 [e]	0.03	0.002 [f]
205-99-2	Benzo(*b*)fluoranthene	0.9 [e]	--- [c]	5 [e]	0.2 [e,f]
207-08-9	Benzo(*k*)fluoranthene	9 [e]	--- [c]	49 [e]	2 [e]
65-85-0	Benzoic acid	3.1E+05 [b]	--- [c]	400 [b,i]	20 [b,i]
50-32-8	Benzo(*a*)pyrene	0.09 [e,f]	--- [c]	8	0.4
111-44-4	Bis(2-chloroethyl)ether	0.6 [e]	0.2 [e,f]	0.0004 [e,f]	2E-05 [e,f]
117-81-7	Bis(2-ethylhexyl)phthalate	46 [e]	31,000 [d]	3,600	180
75-27-4	Bromodichloromethane	10 [e]	3,000 [d]	0.6	0.03
75-25-2	Bromoform	81 [e]	53 [e]	0.8	0.04
71-36-3	Butanol	7,800 [b]	10,000 [d]	17 [b]	0.9 [b]
85-68-7	Butyl benzyl phthalate	16,000 [b]	930 [d]	930 [d]	810 [b]
86-74-8	Carbazole	32 [e]	--- [c]	0.6 [e]	0.03 [e,f]
75-15-0	Carbon disulfide	7,800 [b]	720 [d]	32 [b]	2 [b]
56-23-5	Carbon tetrachloride	5 [e]	0.3 [e]	0.07	0.003 [f]
57-74-9	Chlordane	0.5 [e]	20 [e]	10	0.5
106-47-8	*p*-Chloroaniline	310 [b]	--- [c]	0.7 [b]	0.03 [b,f]
108-90-7	Chlorobenzene	1,600 [b]	130 [b]	1	0.07
124-48-1	Chlorodibromomethane	8 [e]	1,300 [d]	0.4	0.02
67-66-3	Chloroform	100 [e]	0.3 [e]	0.6	0.03
95-57-8	2-Chlorophenol	390 [b]	53,000 [d]	4 [b,i]	0.2 [b,f,i]
218-01-9	Chrysene	88 [e]	--- [c]	160 [e]	8 [e]
72-54-8	DDD	3 [e]	--- [c]	16 [e]	0.8 [e]
72-55-9	DDE	2 [e]	--- [c]	54 [e]	3 [e]
50-29-3	DDT	2 [e]	--- [g]	32 [e]	2 [e]
53-70-3	Dibenz(*a,h*)anthracene	0.09 [e,f]	--- [c]	2 [e]	0.08 [e,f]
84-74-2	Di-*n*-butyl phthalate	7,800 [b]	2,300 [d]	2,300 [d]	270 [b]
95-50-1	1,2-Dichlorobenzene	7,000 [b]	560 [d]	17	0.9
106-46-7	1,4-Dichlorobenzene	27 [e]	--- [g]	2	0.1 [f]
91-94-1	3,3-Dichlorobenzidine	1 [e]	--- [c]	0.007 [e,f]	0.0003 [e,f]
75-34-3	1,1-Dichloroethane	7,800 [b]	1,300 [b]	23 [b]	1 [b]
107-06-2	1,2-Dichloroethane	7 [e]	0.4 [e]	0.02	0.001 [f]
75-35-4	1,1-Dichloroethylene	1 [e]	0.07 [e]	0.06	0.003 [f]
156-59-2	*cis*-1,2-Dichloroethylene	780 [b]	1,200 [d]	0.4	0.02
156-60-5	*trans*-1,2-Dichloroethylene	1,600 [b]	3,100 [d]	0.7	0.03
120-83-2	2,4-Dichlorophenol	230 [b]	--- [c]	1 [b,i]	0.05 [b,f,i]

Table A-1 (continued)

Organics				**Migration to ground water**	
CAS No.	**Compound**	**Ingestion (mg/kg)**	**Inhalation volatiles (mg/kg)**	**20 DAF (mg/kg)**	**1 DAF (mg/kg)**
78-87-5	1,2-Dichloropropane	9 [e]	15 [b]	0.03	0.001 [f]
542-75-6	1,3-Dichloropropene	4 [e]	0.1 [e]	0.004 [e]	0.0002 [e]
60-57-1	Dieldrin	0.04 [e]	1 [e]	0.004 [e]	0.0002 [e,f]
84-66-2	Diethylphthalate	63,000 [b]	2,000 [d]	470 [b]	23 [b]
105-67-9	2,4-Dimethylphenol	1,600 [b]	--- [c]	9 [b]	0.4 [b]
51-28-5	2,4-Dinitrophenol	160 [b]	--- [c]	0.3 [b,f,i]	0.01 [b,f,i]
121-14-2	2,4-Dinitrotoluene	0.9 [e]	--- [c]	0.0008 [e,f]	4E-05 [e,f]
606-20-2	2,6-Dinitrotoluene	0.9 [e]	--- [c]	0.0007 [e,f]	3E-05 [e,f]
117-84-0	Di-*n*-octyl phthalate	1,600 [b]	10,000 [d]	10,000 [d]	10,000 [d]
115-29-7	Endosulfan	470 [b]	--- [c]	18 [b]	0.9 [b]
72-20-8	Endrin	23 [b]	--- [c]	1	0.05
100-41-4	Ethylbenzene	7,800 [b]	400 [d]	13	0.7
206-44-0	Fluoranthene	3,100 [b]	--- [c]	4,300 [b]	210 [b]
86-73-7	Fluorene	3,100 [b]	--- [c]	560 [b]	28 [b]
76-44-8	Heptachlor	0.1 [e]	4 [e]	23	1
1024-57-3	Heptachlor epoxide	0.07 [e]	5 [e]	0.7	0.03
118-74-1	Hexachlorobenzene	0.4 [e]	1 [e]	2	0.1 [f]
87-68-3	Hexachloro-1,3-butadiene	8 [e]	8 [e]	2	0.1 [f]
319-84-6	α-HCH (α-BHC)	0.1 [e]	0.8 [e]	0.0005 [e,f]	3E-05 [e,f]
319-85-7	β-HCH (β-BHC)	0.4 [e]	--- [g]	0.003 [e]	0.0001 [e,f]
58-89-9	γ-HCH (Lindane)	0.5 [e]	--- [c]	0.009	0.0005 [f]
77-47-4	Hexachlorocyclopentadiene	550 [b]	10 [b]	400	20
67-72-1	Hexachloroethane	46 [e]	55 [e]	0.5 [e]	0.02 [e,f]
193-39-5	Indeno(1,2,3-*cd*)pyrene	0.9 [e]	--- [c]	14 [e]	0.7 [e]
78-59-1	Isophorone	670 [e]	4,600 [d]	0.5 [e]	0.03 [e,f]
7439-97-6	Mercury	23 [b,l]	10 [b,i]	2 [i]	0.1 [i]
72-43-5	Methoxychlor	390 [b]	--- [c]	160	8
74-83-9	Methyl bromide	110 [b]	10 [b]	0.2 [b]	0.01 [b,f]
75-09-2	Methylene chloride	85 [e]	13 [e]	0.02 [e]	0.001 [e,f]
95-48-7	2-Methylphenol	3,900 [b]	--- [c]	15 [b]	0.8 [b]
91-20-3	Naphthalene	3,100 [b]	--- [c]	84 [b]	4 [b]
98-95-3	Nitrobenzene	39 [b]	92 [b]	0.1 [b,f]	0.007 [b,f]
86-30-6	*N*-Nitrosodiphenylamine	130 [e]	--- [c]	1 [e]	0.06 [e,f]
621-64-7	*N*-Nitrosodi-*n*-propylamine	0.09 [e,f]	--- [c]	5E-05 [e,f]	2E-06 [e,f]
1336-36-3	PCBs	1 [h]	--- [h]	--- [h]	--- [h]
87-86-5	Pentachlorophenol	3 [e,j]	--- [c]	0.03 [f,i]	0.001 [f,i]
108-95-2	Phenol	47,000 [b]	--- [c]	100 [b]	5 [b]
129-00-0	Pyrene	2,300 [b]	--- [c]	4,200 [b]	210 [b]
100-42-5	Styrene	16,000 [b]	1,500 [d]	4	0.2
79-34-5	1,1,2,2-Tetrachloroethane	3 [e]	0.6 [e]	0.003 [e,f]	0.0002 [e,f]

Table A-1 (continued)

Organics				**Migration to ground water**	
CAS No.	**Compound**	**Ingestion (mg/kg)**	**Inhalation volatiles (mg/kg)**	**20 DAF (mg/kg)**	**1 DAF (mg/kg)**
127-18-4	Tetrachloroethylene	12 [e]	11 [e]	0.06	0.003 [f]
108-88-3	Toluene	16,000 [b]	650 [d]	12	0.6
8001-35-2	Toxaphene	0.6 [e]	89 [e]	31	2
120-82-1	1,2,4-Trichlorobenzene	780 [b]	3,200 [d]	5	0.3 [f]
71-55-6	1,1,1-Trichloroethane	--- [c]	1,200 [d]	2	0.1
79-00-5	1,1,2-Trichloroethane	11 [e]	1 [e]	0.02	0.0009 [f]
79-01-6	Trichloroethylene	58 [e]	5 [e]	0.06	0.003 [f]
95-95-4	2,4,5-Trichlorophenol	7,800 [b]	--- [c]	270 [b,i]	14 [b,i]
88-06-2	2,4,6-Trichlorophenol	58 [e]	200 [e]	0.2 [e.f.i]	0.008 [e,f,i]
108-05-4	Vinyl acetate	78,000 [b]	1,000 [b]	170 [b]	8 [b]
75-01-4	Vinyl chloride	0.3 [e]	0.03 [e]	0.01 [f]	0.0007 [f]
108-38-3	*m*-Xylene	1.6E+05 [b]	420 [d]	210	10
95-47-6	*o*-Xylene	1.6E+05 [b]	410 [d]	190	9
106-42-3	*p*-Xylene	1.6E+05 [b]	460 [d]	200	10

Table A-1 (continued)

Inorganics				Migration to ground water	
CAS No.	**Compound**	**Ingestion (mg/kg)**	**Inhalation fugitive particulate (mg/kg)**	**20 DAF (mg/kg)**	**1 DAF (mg/kg)**
7440-36-0	Antimony	31 [b]	--- [c]	5	0.3
7440-38-2	Arsenic	0.4 [e]	750 [e]	29 [i]	1 [i]
7440-39-3	Barium	5,500 [b]	6.9E+05 [b]	1,600 [i]	82 [i]
7440-41-7	Beryllium	0.1 [e]	1,300 [e]	63 [i]	3 [i]
7440-43-9	Cadmium	78 [b,m]	1,800 [e]	8 [i]	0.4 [i]
7440-47-3	Chromium (total)	390 [b]	270 [e]	38 [i]	2 [i]
16065-83-1	Chromium (III)	78,000 [b]	--- [c]	--- [g]	--- [g]
18540-29-9	Chromium (VI)	390 [b]	270 [e]	38 [i]	2 [i]
57-12-5	Cyanide (amenable)	1,600 [b]	--- [c]	40	2
7439-92-1	Lead	400 [k]	--- [k]	--- [k]	--- [k]
7440-02-0	Nickel	1,600 [b]	13,000 [e]	130 [i]	7 [i]
7782-49-2	Selenium	390 [b]	--- [c]	5 [i]	0.3 [i]
7440-22-4	Silver	390 [b]	--- [c]	34 [b,i]	2 [b,i]
7440-28-0	Thallium	--- [c]	--- [c]	0.7 [i]	0.04 [i]
7440-62-2	Vanadium	550 [b]	--- [c]	6,000 [b]	300 [b]
7440-66-6	Zinc	23,000 [b]	--- [c]	12,000 [b,i]	620 [b,i]

DAF = Dilution and attenuation factor.

[a] Screening levels based on human health criteria only.

[b] Calculated values correspond to a noncancer hazard quotient of 1.

[c] No toxicity criteria available for that route of exposure.

[d] Soil saturation concentration (C_{sat}).

[e] Calculated values correspond to a cancer risk level of 1 in 1,000,000.

[f] Level is at or below Contract Laboratory Program required quantitation limit for Regular Analytical Services (RAS).

[g] Chemical-specific properties are such that this pathway is not of concern at any soil contaminant concentration.

[h] A preliminary remediation goal of 1 mg/kg has been set for PCBs based on *Guidance on Remedial Actions for Superfund Sites with PCB Contamination* (U.S. EPA, 1990) and on EPA efforts to manage PCB contamination.

[i] SSL for pH of 6.8.

[j] Ingestion SSL adjusted by a factor of 0.5 to account for dermal exposure.

[k] A screening level of 400 mg/kg has been set for lead based on *Revised Interim Soil Lead Guidance for CERCLA Sites and RCRA Corrective Action Facilities* (U.S. EPA, 1994).

[l] SSL is based on RfD for mercuric chloride (CAS No. 007487-94-7).

[m] SSL is based on dietary RfD.

Table A-2. Generic SSLs: Default Parameters and Assumptions

Parameter	SSL pathway		Default
	Inhalation	Migration to ground water	
Source Characteristics			
Continuous vegetative cover	●		50 percent
Roughness height	❍		0.5 cm for open terrain; used to derive $U_{t,7}$
Source area (A)	●	❍	0.5 acres (2,024 m^2); used to derive L for MTG
Source length (L)		●	45 m (assumes square source)
Source depth		❍	Extends to water table (i.e., no attenuation in unsaturated zone)
Soil Characteristics			
Soil texture	❍	❍	Loam; defines soil characteristics/ parameters
Dry soil bulk density (ρ_b)	●	●	1.5 kg/L
Soil porosity (n)	●	❍	0.43
Vol. soil water content (θ_w)	●	●	0.15 (INH); 0.30 (MTG)
Vol. soil air content (θ_a)	●	●	0.28 (INH); 0.13 (MTG)
Soil organic carbon (f_{oc})	●	●	0.006 (0.6%, INH); 0.002 (0.2 %, MTG)
Soil pH	❍	❍	6.8; used to determine pH-specific K_d (metals) and K_{oc} (ionizable organics)
Mode soil aggregate size	❍		0.5 mm; used to derive $U_{t,7}$
Threshold windspeed @ 7 m ($U_{t,7}$)	●		11.32 m/s
Meteorological Data			
Mean annual windspeed (U_m)	●		4.69 m/s (Minneapolis, MN)
Air dispersion factor (Q/C)	●		90th percentile conterminous U.S.
Volatilization Q/C	●		68.81; Los Angeles, CA; 0.5-acre source
Fugitive particulate Q/C	●		90.80; Minneapolis, MN; 0.5-acre source
Hydrogeologic Characteristics			
Hydrogeologic setting		❍	Generic (national); surficial aquifer
Dilution/attenuation factor (DAF)		●	20

● Indicates input parameters directly used in SSL equations.
❍ Indicates parameters/assumptions used to develop SSL input parameters.
INH = Inhalation pathway.
MTG = Migration to ground water pathway.

Analysis of Effects of Source Size on Generic SSLs

A large number of commenters on the December 1994 Soil Screening Guidance suggested that most contaminated soil sources were 0.5 acre or less. Before changing this default assumption from 30 acres to 0.5 acre, the Office of Emergency and Remedial Response (OERR) conducted an analysis of the effects of changing the area of a contaminated soil source on generic SSLs calculated for the inhalation and migration to ground water exposure pathways. This analysis includes:

- An analysis of the sensitivity of SSLs to a change in source area from 30 acres to 0.5 acre

- Mass-limit modeling results showing the depth of contamination for a 30-acre source that corresponds to a 0.5-acre SSL.

All equations, assumptions, and model input parameters used in this analysis are consistent with those described in Part 2 of this document unless otherwise indicated. Chemical properties used in the analysis are described in Part 5 of this document.

In summary, the results of this analysis indicate that:

- The SSLs are not particularly sensitive to varying the source area from 30 acres to 0.5 acre. This reduction in source area lowers SSLs for the inhalation pathway by about a factor of 2 and lowers SSLs for the migration to ground water pathway by a factor of 2.9 under typical hydrogeologic conditions.

- Half-acre SSLs calculated for 43 volatile and semivolatile contaminants using the infinite source models correspond to mass-limit SSLs for a 30-acre source uniformly contaminated to a depth of about 1 to 21 meters (depending on contaminant and pathway); the average depth is 8 meters for the inhalation pathway (21 contaminants) and 11 meters for the migration to ground water pathway (43 contaminants).

Sensitivity Analysis. For the inhalation pathway, source area affects the Q/C value (a measure of dispersion), which directly affects the final SSL and is not chemical-specific. Higher Q/C values result in higher SSLs. As shown in Table 3 (Section 2.4.3), the effect of area on the Q/C value is not sensitive to meteorological conditions, with the ratio of a 0.5-acre Q/C to a 30-acre Q/C ranging from 1.93 to 1.96 over the 29 conditions analyzed. Decreasing the source area from 30 acres to 0.5 acre will therefore increase inhalation SSLs by about a factor of 2.

For the migration to ground water pathway, source area affects the DAF, which also directly affects the final SSLs and is not chemical-specific. The sensitivity analysis for the dilution factor is more complicated than for Q/C because increasing source area (expressed as the length of source parallel to ground water flow) not only increases infiltration to the aquifer, which decreases the dilution factor, but also increases the mixing zone depth, which tends to increase the dilution factor. The first effect generally overrides the second (i.e., longer sources have lower dilution factors) except for very thick aquifers (see Section 2.5.7).

The sensitivity analysis described in Section 2.5.7 shows that the dilution model is most sensitive to the aquifer's Darcy velocity (i.e., hydraulic conductivity × hydraulic gradient). For a less conservative Darcy velocity (90th percentile), decreasing the source area from 30 acres to 0.5 acre increased the dilution factor by a factor of 3.1 (see Table 9, Section 2.5.7). For the conditions analyzed, decreasing the source area from 30 acres to 0.5 acre affected dilution factor from no increase to a factor of 4.3 increase. No increase in dilution factor for a 0.5-acre source was observed for the less conservative (higher) aquifer thickness (46 m). In this case the decrease in mixing zone depth balances the decrease in infiltration rate for the smaller source.

Mass-Limit Analysis. The infinite source assumption is one of the more conservative assumptions inherent in the SSL models, especially for small sources. This assumption should provide adequate protection for sources with larger areas than those used to calculate SSLs. To test this hypothesis the SSL mass-limit models (Section 2.6) were used to calculate, for 43 volatile and semivolatile chemicals, the depth at which a mass-limit SSL for a 30-acre source is equal to a 0.5-acre infinite-source SSL.

The mass-limit models are simple mass-balance models that calculate SSLs based on the conservative assumption that the entire mass of contamination in a source either volatilizes (inhalation model) or leaches (migration to ground water model) over the exposure period of interest. These models were developed to correct the mass-balance violation in the infinite source models for highly volatile or soluble contaminants.

Table A-3 presents the results of this analysis. These results demonstrate that 0.5-acre infinite source SSLs are protective of uniformly contaminated 30-acre source areas of significant depth. For the 21 chemicals analyzed for the inhalation pathway, these source depths range up to 21 meters, with an average depth of 8 meters and a standard deviation of 5.7. For the migration to ground water pathway, source depths for 43 contaminants range to 21 meters, with an average of 11 meters and a standard deviation of 5.4.

References

U.S. EPA (Environmental Protection Agency). 1990. *Guidance on Remedial Actions for Superfund Sites with PCB Contamination*. Office of Solid Waste and Emergency Response, Washington, DC. NTIS PB91-921206CDH.

U.S. EPA (Environmental Protection Agency). 1994. *Revised Interim Soil Lead Guidance for CERCLA Sites and RCRA Corrective Action Facilities*. Office of Solid Waste and Emergency Response, Washington, DC. Directive 9355.4-12.

Table A-3.Source Depth where 30-acre[a] Mass-Limit SSLs = 0.5-acre[b] Infinite-Source SSLs[c]

	Source depth (m)	
Chemical	**Inhalation**	**Migration to ground water[c]**
Acetone	NA	21
Benzene	8.1	12
Benzoic acid	NA	21
Bis(2-chloroethyl)ether	0.7	18
Bromodichloromethane	NA	13
Bromoform	0.9	11
Butanol	NA	20
Carbon disulfide	19	11
Carbon tetrachloride	11	6
Chlorobenzene	3.5	6
Chlorodibromomethane	NA	13
Chloroform	8.3	14
2-Chlorophenol	NA	4
1,2-Dichlorobenzene	NA	3
1,4-Dichlorobenzene	NA	3
1,1-Dichloroethane	9.1	15
1,2-Dichloroethane	5.6	18
1,1-Dichloroethylene	15	10
cis-1,2-Dichloroethylene	NA	15
trans-1,2-Dichloroethylene	NA	12
2,4-Dichlorophenol	NA	8
1,2-Dichloropropane	6.2	14
1,3-Dichloropropene	12	12
2,4-Dimethylphenol	NA	7
2,4-Dinitrophenol	NA	21
2,4-Dinitrotoluene	NA	11
2,6-Dinitrotoluene	NA	12
Ethylbenzene	NA	4
Methyl bromide	12	17
Methylene chloride	8.9	18
2-Methylphenol	NA	11
Nitrobenzene	0.5	13
1,1,2,2-Tetrachloroethane	1.6	11
Tetrachloroethylene	8.7	7
Toluene	NA	7
1,1,1-Trichloroethane	NA	9
1,1,2-Trichloroethane	3.4	14
Trichloroethylene	6.8	7
Vinyl acetate	4.6	20

Table A-3. (continued)

Chemical	Source depth (m)	
	Inhalation	Migration to ground water[c]
Vinyl chloride	21	13
m-Xylene	NA	4
o-Xylene	NA	4
p-Xylene	NA	4

NA = Risk-based SSL not available.

[a] Q/C = 35.15; DAF = 10.

[b] Q/C = 68.81; DAF = 20.

[c] Migration to ground water mass-limit analysis based on 70-yr exposure duration and 0.18 m/yr infiltration rate.

APPENDIX B

Route-to-Route Extrapolation of Inhalation Benchmarks

APPENDIX B

Route-to-Route Extrapolation of Inhalation Benchmarks

Introduction

For a number of the contaminants commonly found at Superfund sites, inhalation benchmarks for toxicity are not available from IRIS or HEAST. As pointed out by commenters to the December 1994 *Soil Screening Guidance*, ingestion SSLs tend to be higher than inhalation SSLs for most volatile chemicals with both inhalation and ingestion benchmarks. This suggests that ingestion SSLs may not be adequately protective for inhalation exposure to chemicals that lack inhalation benchmarks.

To address this concern, the Office of Emergency and Remedial Response (OERR) evaluated potential approaches for deriving inhalation benchmarks using route-to-route extrapolation from oral benchmarks (e.g., inhalation reference concentrations [RfCs] from oral reference doses [RfDs]). OERR evaluated Agency initiatives concerning route-to-route extrapolation, including: the potential reactivity of airborne toxicants (e.g., portal-of-entry effects), the pharmacokinetic behavior of toxicants for different routes of exposure (e.g., absorption by the gut versus absorption by the lung), and the significance of physicochemical properties in determining dose (e.g., volatility, speciation). During this process, OERR consulted with staff in the EPA Office of Research and Development (ORD) to identify appropriate techniques and key technical aspects in performing route-to-route extrapolation. The following sections describe OERR's analysis of route-to-route extrapolation and the conclusions reached regarding the use of extrapolated inhalation benchmarks to support inhalation SSLs.

B.1 Extrapolation of Inhalation Benchmarks

The first step taken in considering route-to-route extrapolation of inhalation benchmarks was to compare existing inhalation benchmarks to inhalation benchmarks extrapolated from oral studies. This comparison was important to determine whether a simple route-to-route extrapolation could provide a defensible inhalation benchmark for chemicals lacking appropriate inhalation studies. OERR identified nine chemicals found in IRIS (Integrated Risk Information System) that have verified RfDs and RfCs for noncancer effects, including three chemicals found in the SSL guidance (ethylbenzene, styrene, and toluene). Reference concentrations for inhalation exposure were extrapolated from oral reference doses for adults using the following formula:

$$\text{extrapolated RfC}\ \left(\text{mg}/\text{m}^3\right) = \text{RfD}\ \left(\text{mg}/\text{kg}-\text{d}\right) \times \frac{70\ \text{kg}}{20\ \text{m}^3/\text{d}} \ . \qquad \textbf{(B-1)}$$

It is important to note that dosimetric adjustments were not made to account for respiratory tract deposition efficiency and distribution; physical, biological, and chemical factors; and other aspects of exposure (e.g., discontinuous exposure) that affect uptake and clearance. Consequently, this simple extrapolation method relies on the implicit assumption that the route of administration is irrelevant to the dose delivered to a target organ, an assumption not supported by the principles of dosimetry or pharmacokinetics.

The limited data on noncarcinogens suggest that more volatile constituents tend to have extrapolated RfCs closer to the RfCs developed by EPA (i.e., extrapolated RfC within a factor of 3 of the RfC in IRIS). The less volatile chemicals (e.g., dichlorvos) tend to be below the RfCs developed by EPA workgroups by 1 to 3 orders of magnitude. Although this data set is insufficient to discern trends in extrapolated versus IRIS RfCs, two points are reasonably clear: (1) for some volatile chemicals, route-to-route extrapolation results in inhalation benchmarks reasonably close to the RfC, and (2) as volatility decreases and/or chemical speciation becomes important (e.g., hydrogen sulfide) with respect to environmental chemistry and toxicology, the uncertainty in extrapolated inhalation benchmarks is likely to increase.

For carcinogens, OERR identified 41 chemicals in IRIS for which oral cancer slope factors (CSF_{oral}) and inhalation unit risk factors (URFs) are available, including 23 chemicals covered under the SSL guidance. Unit risk factors for inhalation exposure were extrapolated from oral carcinogenic slope factors for adults using the following formula:

$$\mathrm{URF}\ (\mu g/m^3)^{-1} = \frac{CSF_{oral}\ (mg/kg-d)^{-1}}{70\ kg} \times 20\ m^3/d \times 10^{-3}\ mg/\mu g\ . \tag{B-2}$$

Using the extrapolated URF, risk-specific air concentrations were calculated as a lifetime average exposure concentration as shown in equation B-3:

$$\text{extrapolated air concentration } \mu g/m^3 = \frac{\text{target risk } 10^{-6}}{\mathrm{URF}\ (\mu g/m^3)^{-1}}\ . \tag{B-3}$$

Not surprisingly, the risk-based (i.e., 10^{-6}) air concentrations in IRIS are the same as the air concentrations extrapolated from the CSF_{oral} for 30 of the 41 carcinogenic chemicals evaluated (at one significant figure). Historically, oral and inhalation slope factors have been based on oral studies for chemicals for which pharmacokinetic or portal-of-entry effects were considered insignificant. As a result, route of exposure extrapolations were often included in the development of the carcinogenic slope factors. However, the divergence of extrapolated air concentrations with risk-based (i.e., 10^{-6}) air concentrations in IRIS reflects newer methods in use at EPA that address portal-of-entry effects, dosimetry, and pharmacokinetic behavior. For example, 1,2-dibromomethane has an extrapolated 10^{-6} air concentration that is 2 orders of magnitude below the value in IRIS. This difference is probably attributable to differences in: (1) the endpoint for inhalation exposure (nasal cavity carcinoma) versus oral exposure (squamous cell carcinoma), and/or (2) portal-of-entry effects directly related to deposition physiology and absorption of 1,2-dibromomethane.

B.2 Comparison of Extrapolated Inhalation SSLs with Generic SSLs

Having performed a simple extrapolation of inhalation benchmarks, the next step was to compare the inhalation SSLs (SSL_{inh}) based on extrapolated data to the soil saturation concentrations* (C_{sat}) and generic SSLs for soil ingestion (SSL_{ing}) and ground water ingestion (SSL_{gw}). Table B-1 presents the 50 organic chemicals in the SSL guidance that lack inhalation benchmarks. The table presents oral benchmarks found in IRIS (columns 2 and 3) and extrapolated inhalation benchmarks as

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* The derivation of C_{sat} and its significance is discussed in Section 2.4.4 of this Technical Background Document.

described in Equations B-1 and B-2 (columns 4 and 5). In addition, the table presents volatilization-based SSLs and SSLs based on particulate emissions derived from the extrapolated toxicity values. For each column of extrapolated inhalation SSLs in this table, values are truncated at 1,000,000 mg/kg because the soil concentration cannot be greater than 100 percent (i.e., 1,000,000 ppm).

B.2.1 Comparison of Extrapolated SSLs Based on Volatilization

The extrapolated SSL_{inh} for volatilization (SSL_{inh-v}) was calculated with Equation 4 in Section 2.4 using a chemical-specific volatilization factor (VF). In Table B-1, the SSL_{inh-v} values based on extrapolated inhalation benchmarks (column 6) are compared with the soil saturation concentration (C_{sat}, column 7) and generic migration to ground water SSLs assuming a dilution attenuation factor (DAF) of 20 (SSL_{gw}).

As described in Section 2.4.4, C_{sat} represents the concentration at which soil pore air is saturated with a chemical and maximum volatile emissions are reached. A comparison of the C_{sat} with the extrapolated SSL_{inh-v} values indicates that, for 36 of the 50 contaminants, SSL_{inh-v} exceeds the soil saturation concentration, often by several orders of magnitude. Because maximum volatile emissions occur at C_{sat}, these 36 contaminants are not likely to pose significant risks through the inhalation pathway, and therefore the lack of inhalation benchmarks is not likely to underestimate risk through the volatilization pathway.

For the remaining 14 contaminants with extrapolated SSL_{inh-v} values below C_{sat}, all are above the generic SSL_{gw} values. This analysis suggests that SSLs based on the migration-to-groundwater pathway are likely to be protective of the inhalation pathway as well. However, for sites where groundwater is not of concern, the SSLs based on ingestion may not necessarily be protective of the inhalation pathway. The analysis indicates that the extrapolated inhalation SSLs are below SSLs based on direct ingestion for the following chemicals: acetone, bromodichloromethane, chlorodibromomethane, cis-1,2-dichloroethylene, and *trans*-1,2-dichloroethylene. This analysis supports the **possibility** that the SSLs based on direct ingestion for the listed chemicals may not be adequately protective of inhalation exposures. However, a more rigorous evaluation of the route-to-route extrapolation methods used to derive the toxicity criteria for this analysis is warranted (refer to section B.3).

B.2.2 Comparison of Extrapolated SSLs Based on Particulate Emissions

The extrapolated particulate inhalation SSLs (SSL_{inh-p}) were calculated with Equation 4 in Section 2.4 using the particulate emission factor (PEF) of 1.32×10^9 m^3/kg. Table B-1 compares the SSL_{inh-p} values based on extrapolated benchmarks (column 10) and generic SSLs based on direct ingestion (SSL_{ing}, Column 9). This comparison indicates that the extrapolated SSL_{inh-p} values that are based on the PEF are well above the SSLs for soil ingestion. Thus, ingestion SSLs are likely to be protective of inhalation risks from fugitive dusts from surface soils.

B.3 Conclusions and Recommendations

Based on the results presented in this appendix, OERR reached several conclusions regarding route-to-route extrapolation of inhalation benchmarks for the development of generic inhalation SSLs. First, it is reasonable to assume that, for some contaminants, the lack of inhalation benchmarks may underestimate risks due to inhalation exposure. Of the 17 volatile organics for which both the ingestion and inhalation SSLs are based on IRIS benchmarks, all had inhalation SSLs that were below the ingestion SSLs. Nevertheless, generic SSLs for ground water ingestion (DAF of 20) are lower, often significantly lower, than both extrapolated and IRIS-based inhalation SSLs with the exception of vinyl chloride, which is gaseous at ambient temperatures. Thus, at sites where ground water is of concern, migration to ground water SSLs generally will be protective from the standpoint of inhalation risk. However, if the ground water is not of concern at a site (e.g., if ground water below the site is not potable), the use of SSLs for soil ingestion may not be adequately protective of the inhalation pathway.

Second, the **extrapolated** SSL_{inh} values are not intended to be used as generic SSLs for site investigations; the **extrapolated** inhalation SSLs are useful in determining the potential for inhalation risks but should not be misused as SSLs. Route-to-route extrapolation methods must account for the relationship between physicochemical properties and absorption and distribution of toxicants, the significance of portal-of-entry effects, and the potential differences in metabolic pathways associated with the intensity and duration of inhalation exposure. However, methods required to generate sufficiently rigorous inhalation benchmarks have recently been developed by the ORD. A final guidance document was made available by ORD in November of 1995 that addresses many of the issues critical to the development of inhalation benchmarks described above. The document, entitled *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry* (U.S. EPA, 1994), describes the application of inhalation dosimetry to derive inhalation reference concentrations and represents the current state-of-the-science at EPA with respect to inhalation benchmark development. The fundamentals of inhalation dosimetry are presented with respect to toxicokinetics and the physicochemical properties of chemical contaminants.

Thus, at sites where the migration to ground water pathway is not of concern and a site manager determines that the inhalation pathway may be significant for contaminants lacking inhalation benchmarks, route-to-route extrapolation may be performed using EPA-approved methods on a case-by-case basis. Chemical-specific route-to-route extrapolations should be accompanied by a complete discussion of the data, underlying assumptions, and uncertainties identified in the extrapolation process. Extrapolation methods should be consistent with the EPA guidance presented in *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry*. If a route-to-route extrapolation is found not to be appropriate based on the ORD guidance, the information on extrapolated SSLs may be included as part of the uncertainty analysis of the baseline risk assessment for the site.

Reference

U.S. EPA (Environmental Protection Agency). 1994. *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry.* EPA/600/8-90/066F. Office of Research and Development, Washington, DC.

Table B-1. Comparison of Extrapolated Inhalation SSLs (SSL_{inh}) with Soil Concentrations (C_{sat}), and Migration to Ground Water (SSL_{gw})

	IRIS oral benchmarks		Extrapolated inhalation benchmarks		VF-based SSLs (mg/kg)				PEF-based SSLs (mg/kg)
Compound	RfD (mg/kg-d)	CSF $(mg/kg\text{-}d)^{-1}$	RfC (mg/m^3)	URF $(mg/m^3)^{-1}$	Extrapolated volatilization $SSL_{inh\text{-}v}$	C_{sat}	Generic SSL_{gw} (DAF 20)	Generic SSL_{ing}	Extrapolated particulate $SSL_{inh\text{-}p}$
Acenaphthene	6E-02		2.1E-01		48,000	181	570	4,700	>1,000,000
Acetone	1E-01		3.5E-01		**4,600**	**103,747**	**16**	**7,800**	>1,000,000
Anthracene	3E-01		1.1E+00		860,000	8	12,000	23,000	>1,000,000
Benz*(a)* anthracene		7.3 E-01		2.1E-04	110	22	2	0.9	15,000
Benzo*(b)* fluoranthene		7.3 E-01		2.1E-04	54	11	5	0.9	15,000
Benzo*(k)* fluoranthene		7.3 E-02		2.1E-05	4,600	6	49	9	150,000
Benzo*(a)* pyrene		7.3 E+00		2.1E-03	28	10	8	0.09	1,500
Benzoic acid	4E+00		1.4E+01		>1,000,000	363	400	310,000	>1,000,000
Bis(2-ethylhexyl)phthalate		1.4 E-02		4.0E-06	130,000	30,804	3,600	46	800,000
Bromodichloromethane		6.2 E-02		1.8E-05	**1.14**	**2,981**	**0.6**	**10**	180,000
Butanol	1E-01		3.5E-01		14,000	10,477	17	7,800	>1,000,000
Butyl benzyl phthalate	2E-01		7.0E-01		>1,000,000	928	930	16,000	>1,000,000
Carbazole		2.0 E-02		5.7E-06	1,100	153	0.6	32	560,000
p -Chloroaniline	4E-03		1.4E-02		4,100	2,632	0.7	310	>1,000,000
Chlorodibromomethane		8.4 E-02		2.4E-05	**1.5**	**1,260**	**0.4**	**8**	130,000
2-Chlorophenol	5E-03		1.8E-02		550	53,482	4	390	>1,000,000
Chrysene		7.3 E-03		2.1E-06	3,200	4	160	88	>1,000,000
DDD		2.4 E-01		6.9E-05	820	540	16	3	47,000
DDE		3.4 E-01		9.7E-05	620	3,218	54	2	33,000
Dibenz*(a,h)* anthracene		7.3 E+00		2.1E-03	120	57	2	0.09	1,500
Di-*n* -butyl phthalate	1E-01		3.5E-01		>1,000,000	2,279	2,300	7,800	>1,000,000
3,3'-Dichlorobenzidine,		4.5 E-01		1.3E-04	24	14	0	1	25,000
***cis* -1,2-Dichloroethylene**	1E-02		3.5E-02		**110**	**1,205**	**0.4**	**780**	>1,000,000
***trans* -1,2-Dichloroethylene**	2E-02		7.0E-02		**170**	**3,067**	**0.7**	**1,600**	>1,000,000
2,4-Dichlorophenol	3E-03		1.1E-02		2,500	4,419	1	240	>1,000,000
Diethylphthalate	8E-01		2.8E+00		>1,000,000	1,974	470	63,000	>1,000,000
2,4-Dimethylphenol	2E-02		7.0E-02		19,000	10,656	9	1,600	>1,000,000
2,4-Dinitrophenol	2E-03		7.0E-03		1,000	279	0.3	160	>1,000,000
2,4-Dinitrotoluene		6.8E-01		1.9E-04	4	182	0.0008	0.9	17,000
2,6-Dinitrotoluene		6.8E-01		1.9E-04	4	94	0.0007	0.9	17,000
Di-*n* -octyl phthalate	2E-02		7.0E-02		>1,000,000	9,984	10,000	1,600	>1,000,000
Endosulfan	6E-03		2.1E-02		18,000	7	18	470	>1,000,000
Endrin	3E-04		1.1E-03		2,500	18	1	23	>1,000,000
Fluoranthene	4E-02		1.4E-01		450,000	132	4300	3,100	>1,000,000

Table B-1. Comparison of Extrapolated Inhalation SSLs (SSL_{inh}) with Soil Concentrations (C_{sat}), and Migration to Ground Water (SSL_{gw})

	IRIS oral benchmarks		Extrapolated inhalation benchmarks		VF-based SSLs (mg/kg)				PEF-based SSLs (mg/kg)
Compound	RfD (mg/kg-d)	CSF $(mg/kg\text{-}d)^{-1}$	RfC (mg/m^3)	URF $(mg/m^3)^{-1}$	Extrapolated volatilization $SSL_{inh\text{-}v}$	C_{sat}	Generic SSL_{gw} (DAF 20)	Generic SSL_{ing}	Extrapolated particulate $SSL_{inh\text{-}p}$
Fluorene	4E-02		1.4E-01		75,000	164	560	3,100	>1,000,000
γ-Hexachlorocyclohexane		1.3 E+00		3.7E-04	3.1	44	0.009	0.5	8,600
Indeno*(* 1,2,3-*cd)* pyrene		7.3 E-01		2.1E-04	660	0.5	14	0.9	15,000
Isophorone		9.5 E-04		2.7E-07	720	4,570	0.5	670	>1,000,000
Methoxychlor	5E-03		1.8E-02		74,000	26	160	390	>1,000,000
2-Methylphenol	5E-02		1.8E-01		37,000	16,827	15	3,900	>1,000,000
Naphthalene	4E-02		1.4E-01		8,200	375	84	3,100	>1,000,000
N -Nitrosodiphenylamine		4.9 E-03		1.4E-06	1,000	275	1	130	>1,000,000
N-Nitrosodi-*n* -propylamine		7.0 E+00		2.0E-03	0.1	2,413	0.00005	0.09	1,600
Pentachlorophenol		1.2 E-01		3.4E-05	83	7,121	0.03	3	94,000
Phenol	6E-01		2.1E+00		400,000	22,588	100	47,000	>1,000,000
Pyrene	3E-02		1.1E-01		420,000	85	4,200	2,300	>1,000,000
2,4,5-Trichlorophenol	1E-01		3.5E-01		250,000	11,618	270	7,800	>1,000,000
m -Xylene	2E+00		7.0E+00		45,000	418	210	160,000	>1,000,000
o -Xylene	2E+00		7.0E+00		45,000	413	190	160,000	>1,000,000
p -Xylene	2E+00		7.0E+00		41,000	461	200	160,000	>1,000,000

NR = $SSL_{inh\text{-}v}$ is greater than 1,000,000 ppm (= no volatile inhalation risk at any soil concentration)

Bold indicates where extrapolated SSL_{inh} values are less than SSL values based on direct ingestion.

APPENDIX C

Limited Validation of the Jury Infinite Source and Jury Finite Source Models (EQ, 1995)

LIMITED VALIDATION OF THE JURY INFINITE SOURCE AND JURY REDUCED SOLUTION FINITE SOURCE MODELS FOR EMISSIONS OF SOIL-INCORPORATED VOLATILE ORGANIC COMPOUNDS

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OFFICE OF SOLID WASTE AND EMERGENCY RESPONSE
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SECTION 1

INTRODUCTION

In December 1995, the U.S. Environmental Protection Agency (EPA) Office of Solid Waste and Emergency Response published the Draft Technical Background Document (TBD) for Soil Screening Guidance (U.S. EPA, 1994). This document provides the technical background behind the development of the Soil Screening Guidance for Superfund, and defines the Soil Screening Framework. The framework consists of a suite of methodologies for developing Soil Screening Levels (SSLs) for 107 chemicals commonly found at Superfund sites. An SSL is defined as "a chemical concentration in soil below which there is no concern under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) for ingestion, inhalation, and migration to ground water exposure pathways...." (U.S. EPA, 1994).

The SSL inhalation pathway considers exposure to vapor-phase contaminants emitted from soils. Inhalation pathway SSLs are calculated using air pathway fate and transport models. Currently, the models and assumptions used to calculate SSLs for inhalation of volatiles are updates of risk assessment methods presented in the Risk Assessment Guidance for Superfund (RAGS) Part B (U.S. EPA, 1991). The RAGS Part B methodology employs a reverse calculation of the concentration in soil of a given contaminant that would result in an acceptable risk-level in ambient air at the point of maximum long-term air concentration.

Integral to the calculation of the inhalation pathway SSLs for volatiles, is the soil-to-air volatilization factor (VF) which defines the relationship between the concentration of contaminants in soil and the volatilized contaminants in air. The VF (m^3/kg) is calculated as the inverse of the ambient air concentration at the center of a ground-level, nonbouyant area source of volatile emissions from soil. The equation for calculating the VF consists of two parts: 1) a volatilization model, and 2) an air dispersion model.

The volatilization model mathematically predicts volatilization of contaminants fully incorporated in soils as a diffusion-controlled process. The basic assumption in the mathematical treatment of the movement of volatile contaminants in soils under a concentration gradient is the applicability of the diffusion laws. The changes in contaminant concentration within the soil as well as the loss of contaminant at the soil surface by volatilization can then be predicted by solving the diffusion equation for different boundary conditions.

As noted in the TBD, Environmental Quality Management, Inc. (EQ) under a subcontract to E. H. Pechan conducted a preliminary evaluation of several soil volatilization models for the U.S. EPA Office of Emergency and Remedial Response (OERR) that might be suitable for addressing both infinite and finite sources of emissions (EQ, 1994). The results of this study indicated that simplified analytical solutions are presented in Jury et al. (1984 and 1990) for both infinite and finite emission sources. These analytical solutions are mathematically consistent and use a common theoretical approximation of the effective diffusion coefficient in soil. Under a subcontract with E. H. Pechan for OERR, EQ performed a limited validation of the Jury Infinite Source emission model (Jury et al., 1984, Equation 8) and the Jury Reduced Solution finite source emission model (Jury et al., 1990, Equation B1), hereinafter known as the Jury volatilization models.

This document reports on several studies in which volatilization of contaminants from soils was directly measured and data were obtained necessary to calculate emissions of contaminants using the Jury Infinite Source model and the Jury Reduced Solution finite source model. These data are then compared and analyzed by statistical methods to determine the relative accuracy of each model.

1.1 PROJECT OBJECTIVES

The primary objective of this project was to assess the relative accuracy of the Jury volatilization models using experimental emission flux data from previous studies as a reference data base.

1.2 TECHNICAL APPROACH

The following series of tasks comprised the technical approach for achieving the project objectives:

1. Review the theoretical basis and development of the Jury volatilization models to verify the applicable model boundary conditions and variables, and to document model assumptions and limitations.

2. Perform a literature search and survey (not to exceed nine contacts) for the purpose of determining the availability of acceptable emission flux data from experimental and field-scale measurement studies of volatile organic compound (VOC) emissions from soils. Acceptable data must have undergone proper quality assurance/quality control (QA/QC) procedures.

3. Determine if the emission flux measurement studies referred to in Task No. 2 also provided sufficient site data as input variables to the volatilization models. Again, acceptable variable input data must have undergone proper QA/QC procedures.

4. Review, collate, and normalize emission flux measurement data and volatilization model variable data, and compute chemical-specific emission rates for comparison to respective measured emission rates.

5. Perform statistical analysis of the results of Task No. 4 to establish the extent of correlation between measured and modeled values and perform parametric analysis of key model variables.

SECTION 2

REVIEW OF THE JURY VOLATILIZATION MODELS

The Jury Reduced Solution finite source volatilization model calculates the instantaneous emission flux from soil at time, t, as:

$$J_s = C_o\, e^{-m}\, (D_E/p\ t)^{1/2} \left[1\ - \exp\,(-L^2/4\, D_E\ t)\right] \tag{1}$$

where J_s = Instantaneous emission flux, μg/cm^2 -day

C_o = Initial soil concentration (total volume), μg/cm^3-soil

μ = Degradation rate constant, 1 /day

t = Time, days

D_E = Effective diffusion coefficient, cm^2 /day

L = Depth from the soil surface to the bottom of contamination, cm

and,

$$DE\ =\ \left[(a^{10/3}\ D_g^a\ K_H\ +\ Q1^{10/3}\ D_i^w)/f^{\,2}\right]/(\rho_b\ f_{oc}\ K_{oc}\ +\ Q\ +\ a\,K_H) \tag{2}$$

where D_E = Effective diffusion coefficient, cm^2 /day

a = Soil volumetric air content, cm^3/cm^3

$D_g^{\ a}$ = Gaseous diffusion coefficient in air, cm^2/day

K_H = Henry's law constant, unitless

Θ = Soil volumetric water content, cm^3/cm^3

D_i^w = Liquid diffusion coefficient in pure water, cm^2/day

ϕ = Total soil porosity, unitless

ρ_b = Soil dry bulk density, g/cm^3

f_{oc} = Soil organic carbon fraction

K_{oc} = Organic carbon partition coefficient, cm^3/g.

The model assumes no boundary layer at the soil-air interface, no water flux through the soil, and an isotropic soil column contaminated uniformly to some depth L. The initial and boundary conditions for which Equation 1 is solved are:

$$c\ =\ C_0 \text{ at } t = 0,\ 0\ \le\ x\ \le\ L$$

$$c\ =\ 0 \text{ at } t = 0,\ x\ \succ\ L$$

$$c = 0 \text{ at } t \succ 0,\ x = 0$$

where c and C_o are, respectively, the soil concentration and initial soil concentration (g/cm^3-total volume), x is the distance measured normal to the soil surface (cm), and t is the time (days).

The average flux over time (J_s^{avg}) is computed by integrating the time-dependent flux over the exposure interval.

The Jury Infinite Source volatilization model calculates the instantaneous emission flux from soil at time, t, as:

$$J_s = C_0 \, (D_E/\pi t)^{1/2} \qquad (3)$$

where J_s = Instantaneous emission flux, μg/cm^2-day

C_o = Initial soil concentration (total volume), μg/cm^3-soil

t = Time, days

D_E = Effective diffusion coefficient, cm^2/day (Equation 2).

The model assumes no boundary layer at the soil-air interface, no water flux through the soil, and an isotropic soil column contaminated uniformly to an infinite depth. The boundary conditions for which Equation 3 is solved are:

$$c = C_0 \text{ at } t \geq 0,\ x = \infty$$

$$c = O \text{ at } t > 0,\ x = 0$$

The average flux over time (J_s^{avg}) is calculated as:

$$J_s^{avg} = C_0 \, (4\, D_E \, /\pi t)^{\,1/2} \qquad (4)$$

2.1 FINITE SOURCE MODEL DERIVATION

The Jury Reduced Solution finite source model is derived from the methods presented by Mayer et al. (1974), and Carslaw and Jaeger (1959). Mayer et al. (1974) considered a system where pesticide is uniformly mixed with a layer of soil and volatilization occurs at the soil surface. If diffusion is the only mechanism supplying pesticide to the surface of an isotropic soil column, and if the diffusion coefficient, D_E, is assumed to be constant, the general diffusion equation is:

$$\frac{\partial^2 c}{\partial x^2} - \frac{1}{D_E} \frac{\partial c}{\partial t} = O \qquad (5)$$

where c = Soil concentration, g/cm^3 - total volume

x = Distance measured normal to soil surface, cm

D_E = Effective diffusion coefficient in soil, cm^2/d

t = Time, days.

If the pesticide is rapidly removed by volatilization from the soil surface and is maintained at a zero concentration, the initial and boundary conditions which also allow for diffusion across the lower boundary at x = L are identical to those of Equation 1.

Recognizing the analogy between the heat transfer equation (Fourier's Law) and the transfer of matter under a concentration gradient (Fick's Law), Mayer et al. (1974) employed the heat transfer equation of Carslaw and Jaeger (1959, page 62, Equation 14) to solve the diffusion equation given these initial and boundary conditions as:

$$C = C_o/2)\{2\ \mathrm{erf}\left[x/2(D_E t)^{1/2}\right] - \mathrm{erf}\left[(x - L)/2(D_E t)^{1/2}\right] - \mathrm{erf}\left[(x + L)/2(D_E t)^{1/2}\right]\} \quad (6)$$

The flux is obtained by differentiating Equation 6 with respect to x, determining $\partial c / \partial x$ at x = O. and multiplying by D_E. The result is:

$$J_s = D_E \left[\partial c/\partial x\right]_{x=o} = \left[D_E\ C_o/\ (\pi D_E t)^{1/2}\right]\left[1 - \exp\ (-L^2/4\ D_E t)\right] \quad (7)$$

Note that Equation 7 is equivalent to the Jury Reduced Solution given in Equation 1 with the exception of the first-order degradation expression $(e^{-\mu t})$.

Jury et al. (1983 and 1990) expanded upon the work of Carslaw and Jaeger (1959) and Mayer et al. (1974) by developing an analytical solution for Equation 5 which includes water flux through the soil column and a soil-air boundary layer. In addition, the Jury et al. solution also includes a theoretical approximation of the effective diffusion coefficient (Equation 2) which was not included in Mayer et al. (1974). Given these conditions, the flux equation from Jury et aI (1983) is given as:

$$J_s = -\ D_E\ (\partial c_T/\partial x)\ +\ V_E\ C_T \quad (8)$$

where C_T = Soil total concentration

x = Depth normal to soil surface

V_E = Effective solute convection velocity.

The minus sign is used because the x direction is positive downward.

Given the initial and boundary conditions:

c = C_o at t=0, $0 \leq x \leq L$

c = O at t=0, x > L

c = O at t>0, x = 0

J_s = - hC_G at t>0, x = 0

where h = Transport coefficient across the soil-air boundary layer of thickness d ($h = D_g^a/d$)

C_G = Vapor-phase concentration ($C_G = K_H\ C_I$), The Jury et al. (1983) analytical solution for the volatilization flux is:

$$J_s(t,L) = + \frac{1}{2} C_o \, V_E \left[\operatorname{erfc} \left(\frac{V_E \, t}{2(D_E t)^{1/2}} \right) - \operatorname{erfc} \left(\frac{L + V_E \, t}{2(D_E t)^{1/2}} \right) \right]$$

$$+ \frac{1}{2} \, C_o (2H_E + V_E) \exp \left(\frac{H_E \, (H_E + V_E) t}{D_E} \right) \tag{9}$$

$$x \left[\exp \left(\frac{H_E L}{D_E} \right) \operatorname{erfc} \left(\frac{L + (2H_E + V_E) t}{2(D_E t)^{1/2}} \right) - \operatorname{erfc} \left(\frac{(2H_E + V_E) t}{2(D_E t)^{1/2}} \right) \right]$$

where H_E Is the transport coefficient across the boundary layer divided by the gasphase partition coefficient, $H_E = h / (\rho_b \; f_{oc} \; K_{oc}/K_H + \Theta/K_H + a)$.

Jury et al. (1990) explains that compounds with large values of K_H are insensitive to the thickness of the soil-air boundary layer (i.e., as $H_E \rightarrow \infty$). Therefore, for the case where $H_E \rightarrow \infty$ and in the absence of water flux ($V_E = 0$) Equation 9 is reduced to Equation 1 where the approximation

$$\operatorname{erfc}\,[x] = \frac{1}{(\pi)^{1/2}} \, \frac{e^{-x^2}}{x} \tag{10}$$

is used to expand the error function for large values of x (Carslaw and Jaeger, 1959).

The Jury Reduced Solution given in Equation 1 is therefore a reduced form of the analytical solution given in Equation 9 for the conditions of zero water flux and no soil-air boundary layer. As such, the Jury Reduced Solution (discounting degradation) is equivalent to the Mayer et al. (1974) solution for diffusion across both the upper and lower boundaries (Equation 7).

2.2 INFINITE SOURCE MODEL DERIVATION

The Jury Infinite Source volatilization model (Equation 3) is derived from Mayer et al. (1974) Equations 3 and 4. Mayer et al. (1974) employed the heat transfer equation of Carslaw and Jaeger (19SS, page 97, Equation 8) to solve the diffusion equation given the boundary conditions:

$$c = C_o \text{ at } t = 0, \; 0 \le x \le L$$

$$c = 0 \text{ at } t \succ 0, \; x = 0$$

$$\partial c / \partial x = 0 \text{ at } x = L$$

The Mayer et al. (1974) solution for the volatilization flux is:

$$J_s = D_E \left[\partial c / \partial x \right]_{x=0} = D_E \, C_o / (\pi \, D_E t)^{1/2} \left[1 + 2 \sum_{n=1}^{\infty} (-1)^n \exp(-n^2 L^2 / D_E t) \right] \tag{11}$$

Therefore, Equation 11 is the analytical solution for a finite emission source, but accounts only for diffusion across the upper boundary.

The summation expression in Equation 11 decreases with increasing L and decreasing D_E and t. If this term is small enough to be negligible, Equation 11 reduces to:

$$J_s = D_E C_o / (\pi D_E t)^{1/2} \tag{12}$$

Use of Equation 12 will result in less than 1 percent error if $t < L^2/18.4\ D_E$ (Mayer et al., 1974) .

Jury et al. (1984 and 1990) gave the solution for the semi-infinite case in Equation 3 where

$C = C_o$ at $t \geq 0,\ x = \infty$ as:

$$J_s = C_o (D_E / \pi\ t)^{1/2}$$

Equation 3 is equivalent to the semi-infinite solution of Mayer et al. (1974) as given in Equation 12 and provides a bounding estimate of the maximum volatilization flux but does not account for source depletion. As with Equation 12, use of Equation 3 on a finite system will result in less than 1 percent error if $t < L^2/18.4\ D_E$. For the purposes of calculating SSLs based on volatilization from soils, let t be set equal to the exposure interval. If $t < L^2/18.4\ D_E$, Equation 1 should be used to calculate the volatilization factor. As an alternative, an estimate of the average emission flux over the exposure interval, $<J_s>$, can be obtained from a simple mass balance:

$$< J_s > = C_o\ L/t \tag{13}$$

where C_o = Initial soil concentration (total volume), µg/cm^3-soil

L = Depth from soil surface to the bottom of contamination, cm

t = Exposure interval, days.

2.3 SUMMARY OF MODEL ASSUMPTIONS AND LIMITATIONS

The Jury Reduced Solution finite source volatilization model is analogous to the mathematical solution for heat flow in a solid such that the region $0 < x < L$ is initially at constant temperature, the region $x > L$ is at zero, and the surface $x = 0$ is maintained at zero for $t > 0$ (Carslaw and Jaeger, 1959). As such, the model's applicability to diffusion processes is limited to the initial and boundary conditions upon which the model is derived. The following represents the major model assumptions for these conditions:

1. Contamination is uniformly incorporated from the soil surface to depth L.
2. The soil column is isotropic to an infinite depth (i.e., uniform bulk density, soil moisture content, porosity and organic carbon fraction).
3. Liquid water flux is zero through the soil column (i.e., no leaching or evaporation).
4. No soil-air boundary layer exists.
5. The soil equilibrium liquid-vapor partitioning (Henry's law) is instantaneous.
6. The soil equilibrium adsorption isotherm is instantaneous, linear, and reversible.

7. Initial soil concentration is in dissolved form (i.e., no residual-phase contamination).

8. Diffusion occurs simultaneously across the upper boundary at x = 0 and the lower boundary at x = L.

The model is therefore limited to surface contamination extending to a known depth and cannot account for subsurface contamination covered by a layer of clean soil. Also, the model does not consider mass flow of contaminants due to water movement in the soil nor the volatilization rate of nonaqueous-phase liquids (residuals). Finally, the model does not account for the resistance of a soil-air boundary layer for contaminants with low Henry's law constants.

The Jury Infinite Source volatilization model is analogous to the mathematical solution for heat flow in a semi-infinite solid. The major model assumptions are the same as those of the Jury Reduced Solution finite source model except that the contamination is assumed to be uniformly incorporated from the soil surface to an infinite depth, and that diffusion occurs only across the upper boundary.

In general, both models describe the vapor-phase diffusion of the contaminants to the soil surface to replace that lost by volatilization to the atmosphere. Each model predicts an exponential decay curve over time once equilibrium is achieved. In actuality, there is a high initial flux rate from the soil as surface concentrations are depleted. The lower flux rate characteristics of the latter portion of the decay curve are thus determined by the rate at which contaminants diffuse upward. This type of desorption curve has been well documented in the literature. It is important to note that both models do not account for the high initial rate of volatilization before equilibrium is attained and will tend to underpredict emissions during this period. Finally, each model is most applicable to single chemical compounds fully incorporated into isotropic soils. Effective solubilities and activity coefficients in multicomponent systems are not addressed in the determination of the effective diffusion coefficient nor is the effect of nonlinear soil adsorption and desorption isotherms. However, because of the complexities involved with theoretical solutions to these effects, their contribution to model accuracy is difficult to predict, especially in multicomponent systems.

SECTION 3

MODEL VALIDATION

To achieve the project objective, EQ executed a literature search and a survey of professional environmental investigation/research firms as well as regulatory agencies to obtain experimental and field data suitable for comparing modeled emissions with actual emissions. The literature search uncovered several papers and bench-scale experimental studies concerned with the volatilization and vapor density of pesticides and chlorinated organics incorporated in soils (Farmer et al., 1972, 1974, and 1980; Spencer and Cliath, 1969 and 1970; Spencer, 1970; and Jury et al., 1980).

3.1 VALIDATION OF THE JURY INFINITE SOURCE MODEL

From the literature search, one bench-scale study was found that approximated the boundary conditions of the Jury Infinite Source model and met the data requirements for this project, Farmer et al., (1972). The Farmer et al. (1972) study reports the experimental emissions of lindane (1,2,3,4,5,6-hexachlorocyclohexane, gamma isomer) and dieldrin (1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4-endo, exo-5, 8-dimethanonapthalene) incorporated in Gila silt loam.

The objective of the survey of professional firms and regulatory agencies was to find pilot-scale or field-scale studies of volatilization of organic compounds using the U.S. EPA emission isolation flux chamber. The candidate flux chamber studies must also have provided adequate data for input to the volatilization models.

Flux chamber studies were chosen to provide pilot-scale or field-scale measurement data needed for model validation. Flux chambers have been widely used to measure flux rates of VOCs and inorganic gaseous pollutants from a wide variety of sources. The flux chamber was originally developed by soil scientists to measure biogenic emissions of inorganic gases and their use dates back at least two decades (Hill et al., 1978). In the early 1980's, EPA became interested in this technique for estimating emission rates from hazardous wastes and funded a series of projects to develop and evaluate the flux chamber method. The initial work involved the development of a design and approach for measuring flux rates from land surfaces. A test cell was constructed and parametric tests performed to assess chamber design and operation (Kienbusch and Ranum, 1986 and Kienbusch et al., 1986). A series of field tests were performed to evaluate the method under field conditions (Radian Corporation, 1984 and Balfour, et al., 1984). A user's guide was subsequently prepared summarizing guidance on the design, construction, and operation of the EPA recommended flux chamber (Keinbusch, 1985). The emission isolation flux chamber is presently considered the preferred in-depth direct measurement technique for emissions of VOCs from land surfaces (EPA, 1990).

EQ contacted several environmental consulting firms as well as State and local agencies. In addition, the EPA data base of emission flux measurement data was reviewed (EPA, 1991a). Although several flux measurement studies were found, only one applicable study was identified with adequate QA/QC documentation and the necessary input data for the Jury Infinite Source model (Radian Corporation, 1989).

From Farmer et al. (1972) the influence of pesticide vapor pressure on volatilization was measured by comparing the volatilization from Gila silt loam of dieldrin with that of lindane. Volatilization of dieldrin and lindane was measured in a closed airflow system by collecting the volatilized insecticides in ethylene glycol traps. Ten grams of soil were treated with either 5 or 10 μg/g of C-14 tagged insecticide in hexane. The hexane was evaporated by placing the soils in a fume hood overnight. Sufficient water was then added to bring the initial soil water content to 10 percent. For the volatilization studies, the treated soil was placed in an aluminum pan 5 mm deep, 29 mm wide, and 95 mm long. This produced a bulk density of 0.75 g/cm^3. The aluminum pan was then introduced into a 250 mL bottle which served as the volatilization chamber. A relative humidity of 100 percent was maintained in the incoming air stream to prevent water evaporation from the soil surface. Air flow was maintained at 8 mL/s equivalent to approximately 0.018 miles per hour. The temperature was maintained at 30°C. The soil was a Gila silt loam, which contained 0.58 percent organic carbon.

The volatilized insecticides were trapped in 25 mL of ethylene glycol. Insecticides were extracted into hexane and anhydrous sodium sulfate was added to the hexane extract to remove water. Aliquots of the dried hexane were analyzed for lindane and dieldrin using liquid scintillation. The extraction efficiencies for lindane and dieldrin were 100 and 95 percent, respectively. The concentrations of volatilized compounds were checked using gas-liquid chromatography. All experiments were run in duplicate.

To ensure that the initial soil concentrations of lindane and dieldrin were in dissolved form, the saturation concentration (mg/kg) of both compounds under experimental conditions was calculated using the procedures given in U.S. EPA (1994):

$$C_{sat} = \frac{S}{\rho_b} (f_{oc}\, K_{oc}\, \rho_b + \Theta + K_H a) \tag{14}$$

where S is the pure component solubility in water. C_{sat} for lindane and dieldrin were calculated to be 34 mg/kg and 12 mg/kg, respectively. Therefore, the initial soil concentrations of 10 and 5 mg/kg were below saturation for both compounds.

Table 1 gives the values of each variable employed to calculate the emissions of lindane and dieldrin using the Jury Infinite Source volatilization model (Equation 3). The potential for loss of contaminant at the lower boundary at each time-step was checked to see if $t > L^2/18.4\ D_E$. If this condition was true at any time-step, the boundary conditions of the infinite source model were violated. In such a case, emissions were also calculated using the finite source model of Mayer et al. (1974) as presented in Equation 11. The difference between the predictions of both models were compared at each time-step and a percent error was calculated for the infinite source model. The instantaneous emission flux values predicted by Equation 3 and Equation 11 (where applicable) were plotted against the measured flux values for dieldrin and lindane at both 5 and 10 ppmw.

Figure 1 shows the comparison of the predicted and measured values of dieldrin at an initial soil concentration of 5 ppmw. For dieldrin, the boundary conditions of the infinite source model were not violated until the last time-step. A best curve was fit to both the measured and predicted values. As expected, both curves indicate an exponential decrease in emissions with time.

The ratio of the modeled emission flux to the measured emission flux was determined as a measure of the relative difference between the modeled and measured values. The natural log of this ratio was then analyzed by using a standard paired Student's t-test. This analysis is equivalent to assuming a lognormal distribution for the emission flux and analyzing the logtransformed data for differences between modeled and measured values.

TABLE 1.
VOLATILIZATION MODEL INPUT VALUES FOR LINDANE AND DIELDRIN

Variable	Symbol	Units	Value	Reference/Equation
Initial soil concentration	C_o	mg/kg	5 and 10	Farmer et al. (1972)
Soil depth	L	cm	0.5	Farmer et al. (1972)
Soil dry bulk density	ρ_b	g/cm^3	0.75	Farmer et al. (1972)
Soil particle density	ρ_s	g/cm^3	2.65	U.S. EPA (1988)
Gravimetric soil moisture content	w	percent	10	Farmer et al. (1972)
Water-filled soil porosoty	Θ	cm^3/cm^3	0.075	$w\rho_s$
Total soil porosity	ϕ	cm^3/cm^3	0.717	$1-(\rho_b/\rho_s)$
Air-filled soil porosity	a	cm^3/cm^3	0.642	ϕ - Θ
Soil organic carbon	f_{oc}	fraction	0.0058	Farmer et al. (1972)
Organic carbon partition coefficient	K_{oc}	cm^3/g	1380	U.S. EPA (1994)
Diffusivity in air (Lindane)	D_g^a	cm^2/d	1521	U.S. EPA (1994)
Diffusivity in air (Dieldin)	D_g^a	cm^2/d	1080	U.S. EPA (1994)
Diffusivity in water (Lindane)	D_i^w	cm^2/d	0.480	U.S. EPA (1994a)
Diffusivity in water (Dieldrin)	D_i^w	cm^2/d	0.410	U.S. EPA (1994a)
Henry's law constant (Lindane)	K_H	unitless	1.40 E-04	U.S. EPA (1994)
Henry's law constant (Dieldrin)	K_H	unitless	2.75 E-06	U.S. EPA (1994)
Degradation rate constant (Lindane and Dieldrin)	μ	1/day	0	Default to eliminate effects of degradation

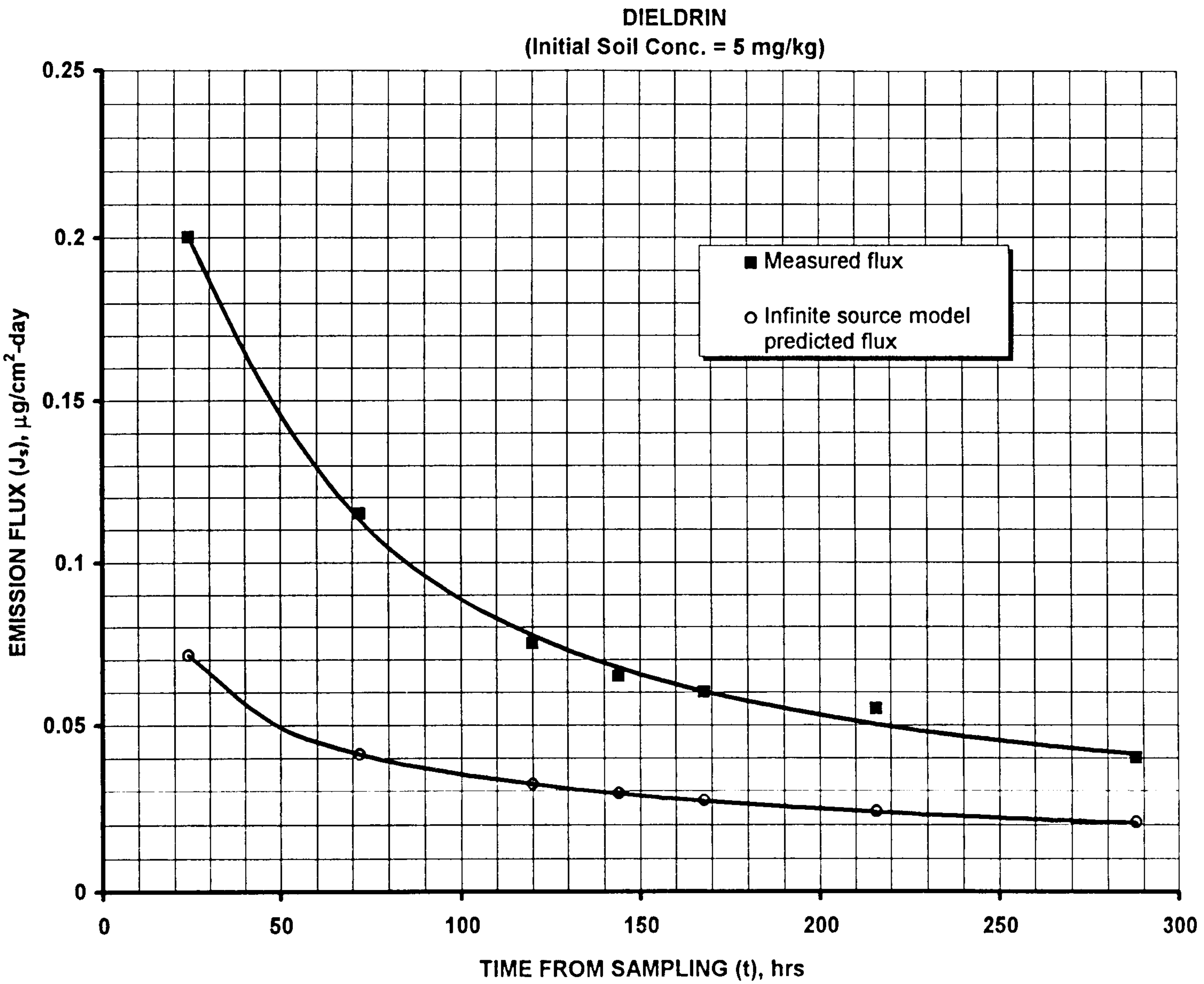


Figure 1
Predicted And Measured Emission Flux Of Dieldrin Versus Time (C_o = 5 ppmw)

The data were also analyzed by using standard linear regression techniques (Figure 2). Again, the data were assumed to follow a lognormal distribution. A simple linear regression model was fit to the log-transformed data and the Pearson correlation coefficient was determined. The Pearson correlation coefficient is a measure of the strength of the linear association between the two variables.

From a limited population of four observations, the correlation coefficient was calculated to be 0.994 with a mean ratio of modeled-to-measured values of 0.42. The actual significance (p-value) of the paired Student's t-test was $p = 0.0001$. The lower and upper confidence limits were calculated to be 0.38 and 0.48, respectively. On average, this indicates that at the 95 percent confidence limit, the modeled emission flux is between 0.38 and 0.48 times the measured emission flux.

Figure 3 shows the modeled and measured flux values of dieldrin at an initial soil concentration of 10 ppmw, while Figure 4 shows the relationship of the log-transformed data and the upper and lower confidence limits. At 10 ppmw, the correlation coefficient was 0.974 with a mean ratio of 0.45, p-value of 0.0001, and a 95 percent confidence interval of 0.37 to 0.54.

As can be seen from Figures 1 and 3, the model underpredicts the emissions during the initial stages of the experiment. This is to be expected in that during this phase, contaminant is evaporating from the soil surface. The apparent discrepancy between measured and predicted values decreases with time as equilibrium is achieved and diffusion becomes the rate-limiting factor.

For lindane, the boundary conditions of the infinite source model were violated after the first time-step (i.e., $t > L^2/18.4\ D_E$ at 24 hours). Therefore, the Mayer et al. (1974) finite source model was used to derive a percent error at each succeeding timestep. At an initial soil concentration of 5 ppmw, the infinite source model predicted 114 percent total mass loss of the finite source model over the entire time span of the experiment. At a concentration of 10 ppmw, the infinite source model predicted 107 percent total mass loss of the finite source model.

Figures 5 and 6 show the comparison of modeled to measured values of lindane at initial soil concentrations of 5 and 10 ppmw, respectively. Likewise, Figures 7 and 8 show the comparisons of the log-transformed data. At an initial soil concentration of 5 ppmw, the correlation coefficient between modeled and measured values was 0.997 with a mean modeled-to-measured ratio of 0.81, a p-value of 0.3281, and a 95 percent confidence interval of 0.46 to 1.44. At an initial soil concentration of 10 ppmw, the correlation coefficient was calculated to be 0.998, the mean ratio 0.73, the p-value 0.1774, and the confidence interval 0.41 to 1.28.

The p-values for dieldrin are considerably lower than those of lindane. This is due to the very narrow confidence interval around the modeled values. In the case of dieldrin, Equation 3 did not predict a loss of contaminant at the lower boundary until the last time-step (i.e., $t > L^2/18.4\ D_E$ at 12 days). This results in a nearly perfect straight line when the log-transformed data are plotted. For dieldrin, therefore, Equations 3 and 11 predict identical values until the last timestep.

Table 2 summarizes statistical analysis for the bench-scale comparative validation of the Jury Infinite Source volatilization model. In general, the data support good agreement between modeled and measured values and show relatively narrow confidence intervals and high correlation coefficients.

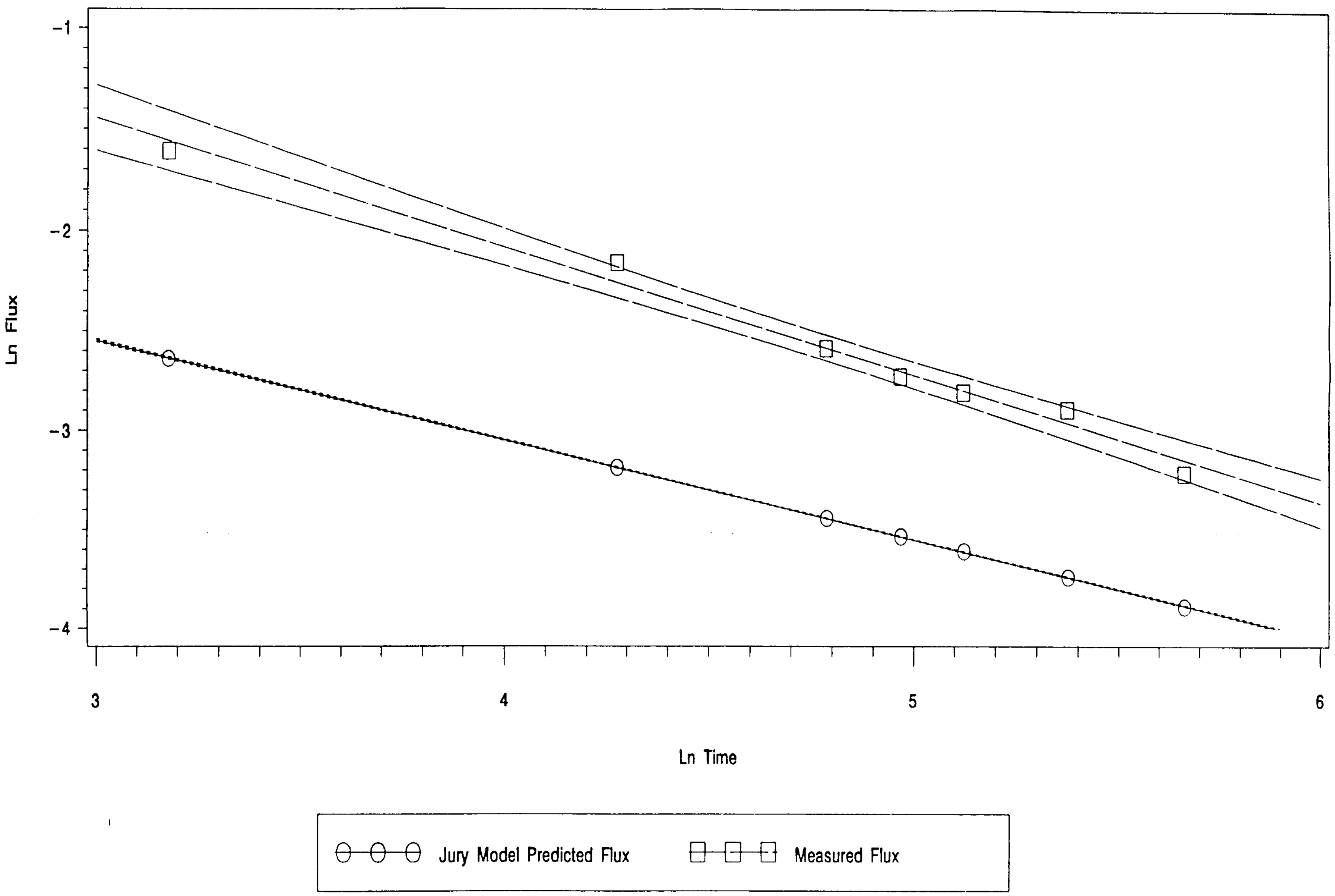


Figure 2
Predicted And Measured Emission Flux Of Dieldrin Versus Time (C_o = 10 ppmw)

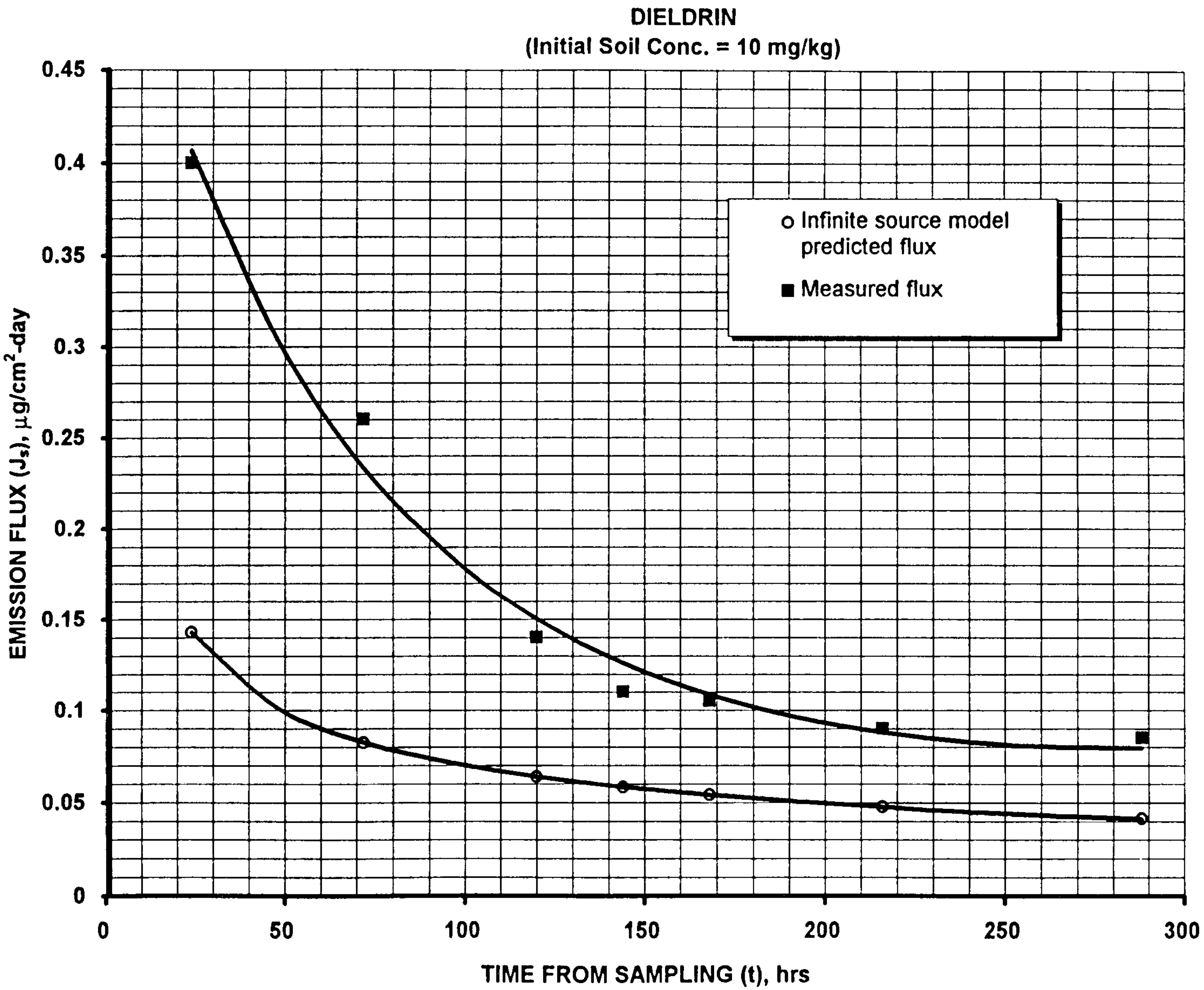


Figure 3
Predicted And Measured Emission Flux Of Dieldrin Versus Time (C_o = 10 ppmw)

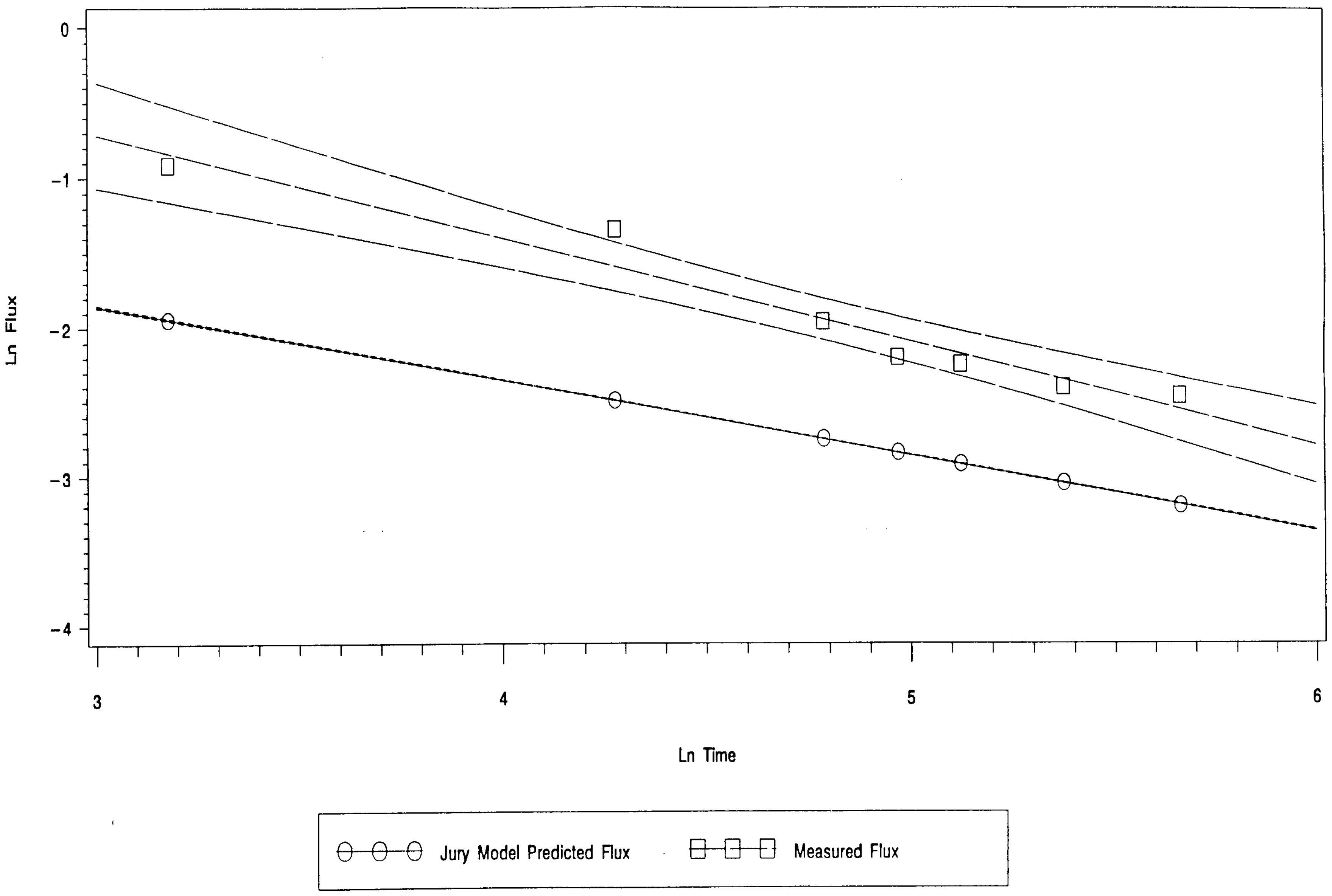


Figure 4
Comparison Of Log-Transformed Modeled And Measured Emission Flux Of Dieldrin (C_o = 10 ppmw)

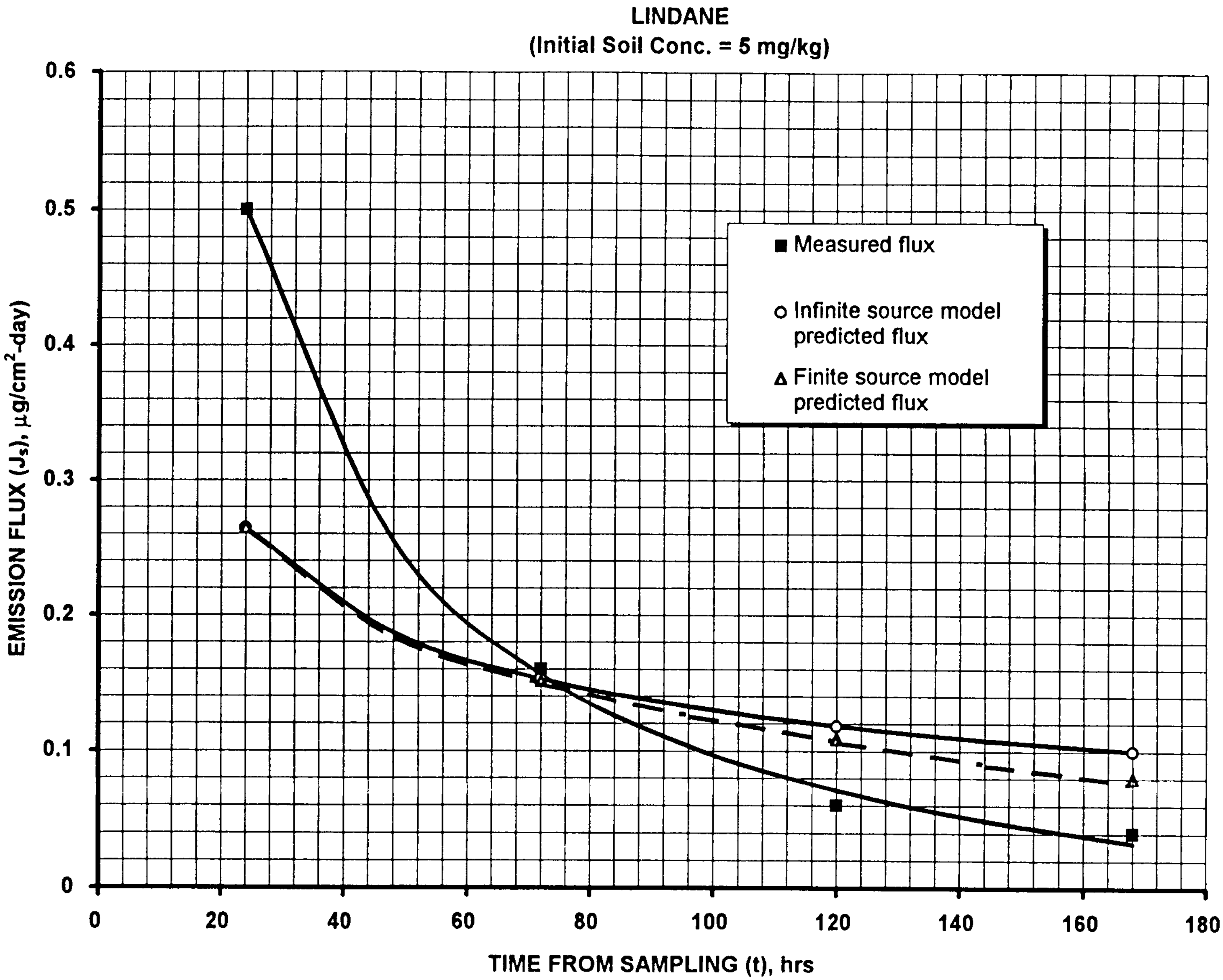


Figure 5
Predicted And Measured Emission Flux Of Lindane Versus Time (Co = 5 ppmw)

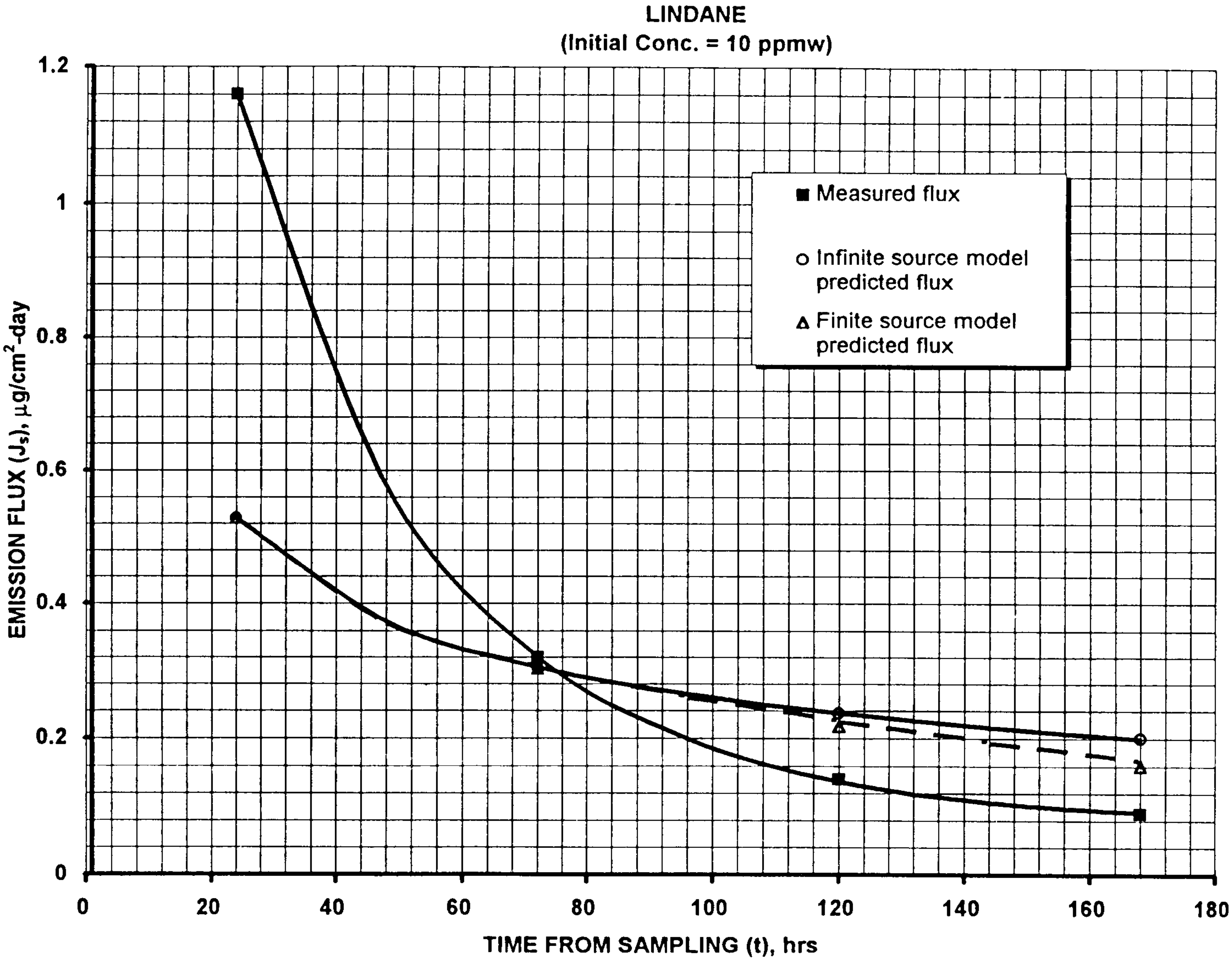


Figure 6
Predicted And Measured Emission Flux Of Lindane Versus Time (C_o = 10 ppmw)

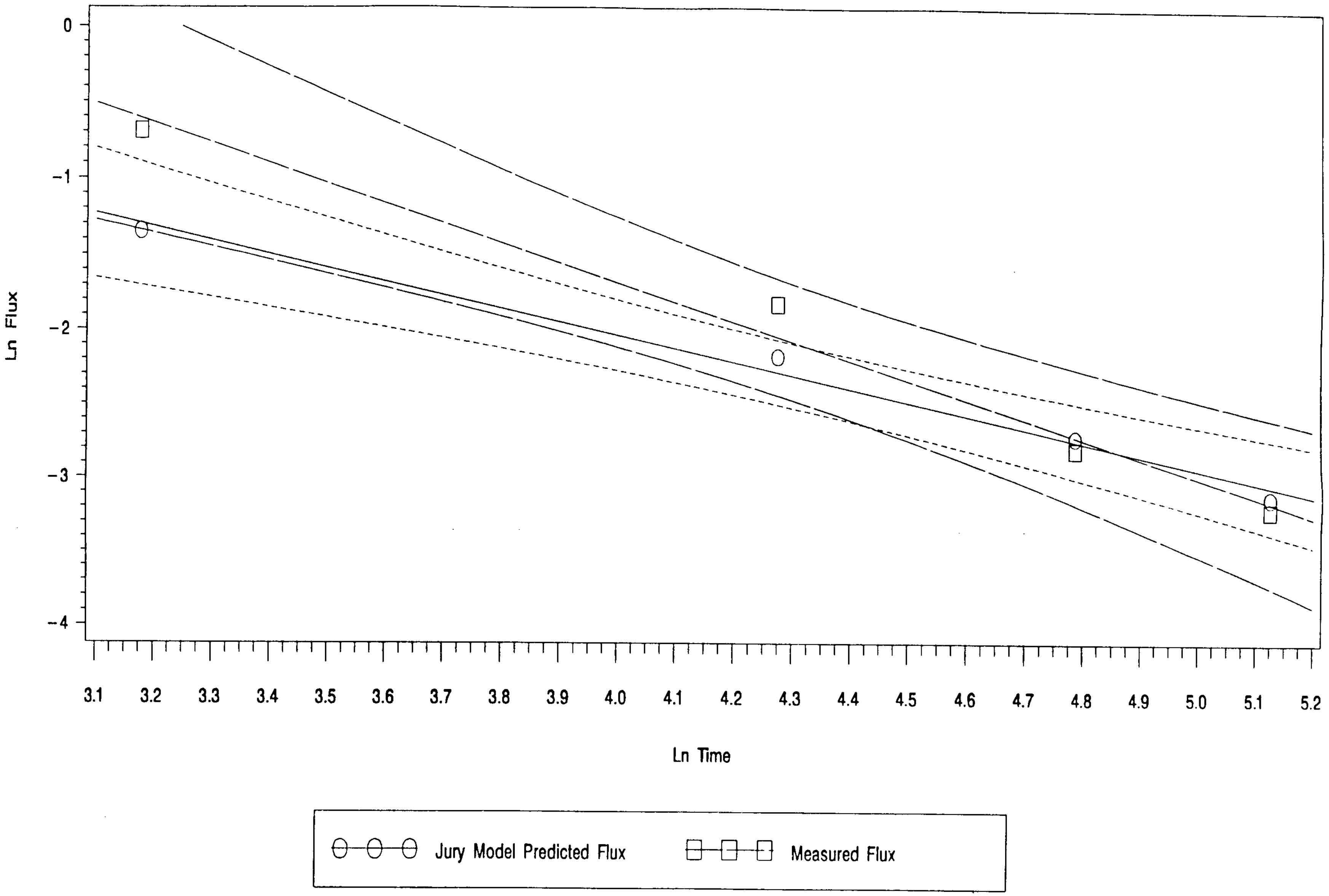


Figure 7
Comparison Of Log-Transformed Modeled And Measured Emission Flux Of Lindane (C_o = 5 ppmw)

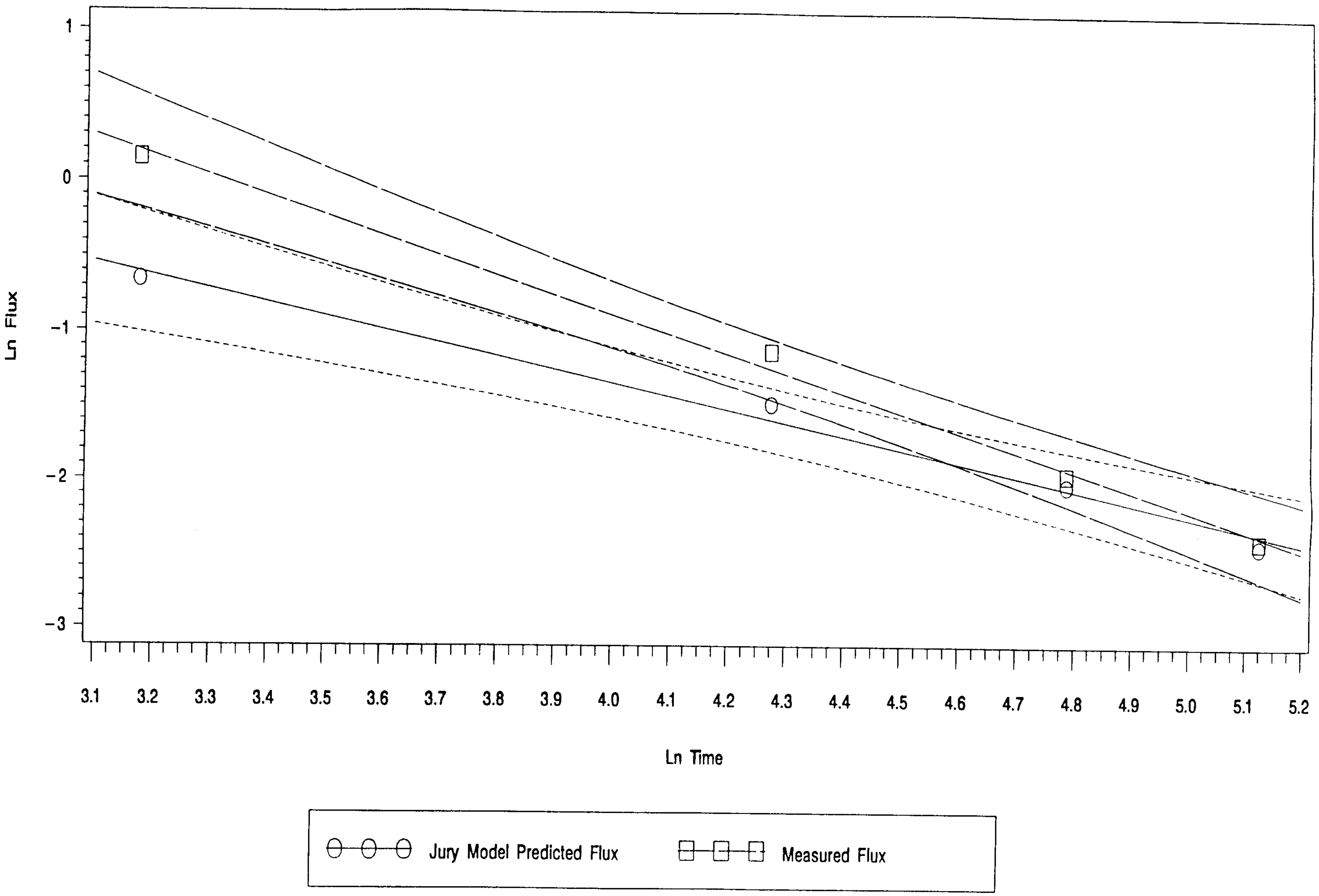


Figure 8
Comparison Of Log-Transformed Modeled And Measured Emission Flux Of Lindane (C_o = 10 ppmw)

TABLE 2.
SUMMARY OF THE BENCH-SCALE VALIDATION OF THE JURY INFINITE SOURCE MODEL

Chemical	N	Correlation coefficient	Mean ratio: Modeled-to-measured	p-value	95% confidence interval
Lindane (5 ppmw)	4	0.997	0.81	0.3281	(0.46, 1.44)
Lindane (10 ppmw)	4	0.998	0.73	0.1774	(0.41, 1.28)
Dieldrin (5 ppmw)	7	0.994	0.42	0.0001	(0.38, 0.48)
Dieldrin (10 ppmw)	7	0.974	0.45	0.0001	(0.37, 0.54)

Appendix A contains the spreadsheet calculations for the bench-scale validation of the Jury Infinite Source volatilization model.

From Radian Corporation (1989), a pilot-scale study was designed to determine how different treatment practices affect the rate of loss of benzene, toluene, xylenes, and ethylbenzene (BTEX) from soils. The experiment called for construction of four piles of loamy sand soil, each with a volume of approximately 4 cubic yards (7900 pounds), a surface area of 8 square meters, and a depth of 0.91 meters. Each test cell was lined with an impermeable membrane and the soil in each cell was sifted to remove particles larger than three-eighth inch in diameter. The contaminated soil for each pile was prepared in batches using 55-gallon drums. In the "high level" study, each soil batch was brought to 5 percent moisture content and 6 liters of gasoline added. Additional water was then added to bring the soil to 10 percent moisture by weight. The drums were capped and sat undisturbed overnight. The drums were then opened the next day and shoveled into the test cell platform. Twenty-two soil batches were prepared for each soil pile. Each batch consisted of 360 pounds of soil and 6.0 liters of fuel. Therefore, each soil pile contained 7900 pounds of soil and 132 liters of gasoline. Each soil pile was then subjected to one of the following management practices:

- A control pile that was not moved or treated
- An "aerated" or "mechanically mixed" pile
- A soil pile simulating soil venting or vacuum extraction
- A soil pile heated to 38°C.

Losses due to volatilization during the mixing and transfer process and during a 28 hour holding time in the test bed before initial sampling reduced the residual BTEX in soil. For the purpose of this validation study, however, these losses caused initial soil concentrations of benzene, toluene, and ethylbenzene to be below or within a factor of two of their respective single component saturation concentrations. Because the mixed pile, vented pile, and heated pile were subject to mechanical disturbances or thermal treatment, only the control pile data were used in this study.

In general, the test schedule called for collection of soil samples and air emission loss measurements during the first, sixth, and seventh weeks Soil samples were collected randomly within specified grid areas by composite core collection to the maximum depth of the pile. Emission losses were measured similarly using an emission isolation flux chamber as specified in Kienbusch (1985). Only data for which soil samples and flux chamber measurements were taken on the same day were used for this study.

Analysis of BTEX in soil samples was accomplished by employing the EPA 5030 extraction method and the EPA 8020 analytical method. The BTEX method was modified to reduce the sample hold time to one day in an effort to improve the accuracy of the method. Five soil samples were submitted in duplicate. The relative percent differences (RPD) ranged from 8.0 to 48.9 percent. The average RPD for the five samples was 26.8 percent. In addition, EPA QC sample analysis indicated average percent recoveries ranging from 89 percent for m-xylene to 119 percent for toluene. The pooled coefficient of variation (CV) for all the BTEX analysis was 10.5 percent. Spiked sample recoveries (eight samples) ranged from 75 percent for m-xylene to 168 percent for toluene. The average spike recoveries ranged from 108 percent for benzene to 146 percent for toluene. Finally, both system blanks and reagent blanks indicated no contamination was found in the analytical system.

It should be noted that the standard method used for BTEX analysis was observed to have contributed to the variabilities in soil concentrations. The EPA acceptance criteria based on 95 percent confidence intervals from laboratory studies are roughly 30 to 160 percent for the BTEX compounds during analysis of water samples. The necessary extraction step for soil samples would increase this already large variability.

Analysis of vapor-phase organic compounds via the emission isolation flux chamber was accomplished using a gas chromatograph (GC). Gas samples were collected from the flux chamber in 100 mL, gas-tight syringes and analyzed by the GC in laboratory facilities adjacent to the test site. During the study, a multicomponent standard was analyzed daily to assess the precision and daily replication of the analytical system. The results of the analysis indicated a good degree of reproducibility with coefficients of variation ranging from 5.1 to 16.3 percent.

From these data, instantaneous emission fluxes were calculated for benzene, toluene, and ethylbenzene corresponding to each time period at which flux chamber measurements were made. Table 3 gives the values of each variable employed to calculate emissions of each compound using the Jury Infinite Source model and the Mayer et al. (1974) finite source model. Appendix A contains the spreadsheet data for benzene, toluene, and ethylbenzene at initial soil concentrations of 110 ppm, 880 ppm, and 310 ppm, respectively.

It should be noted that the fraction of soil organic carbon (f_{oc}) was not available from Radian (1989). For this reason, the default value for f_{oc} of 0.006 from U.S. EPA (1994) was used for all calculations.

Figures 9, 10, and 11 show the comparison of modeled and measured emission fluxes of benzene, toluene, and ethylbenzene, respectively. The Radian Corporation study noted that the second measured value in each figure represented a data outlier, possibly due to the formation of a soil fissure, reducing the soil path resistance and increasing the emission flux.

Table 4 presents the results of the statistical analysis of the comparison of modeled and measured values. For both benzene and ethylbenzene, measured values were below the detection limits after the fifth observation; measured values for toluene were below the detection limit after the seventh observation.

TABLE 3.
VOLATILIZATION MODEL INPUT VARIABLES FOR BENZENE, TOLUENE, AND ETHYLBENZENE

Variable	Symbol	Units	Value	Reference/Equation
Initial soil concentration	C_o	mg/kg		Radian (1989)
- benzene			110	
- toluene			880	
- ethylbenzene			310	
Soil Depth	L	cm	91	Radian (1989)
Soil dry bulk density	ρ_b	g/cm^3	1.5	Radian (1989)
Soil particle density	ρ_s	g/cm^3	2.65	U.S. EPA (1988)
Gravimetric soil moisture content	w	percent	10	Radian (1989)
Water-filled soil porosoty	Θ	cm^3/cm^3	0.150	$w\rho_b$
Total soil porosity	ϕ	cm^3/cm^3	0.434	$1-(\rho_b/\rho_s)$
Air-filled soil porosity	a	cm^3/cm^3	0.284	$\phi - \Theta$
Soil organic carbon	f_{oc}	Fraction	0.006	U.S. EPA (1994) default value
Organic carbon partition coefficient	K_{oc}	cm^3/g		
- benzene			57	U.S. EPA (1994)
- toluene			131	U.S. EPA (1994)
- ethylbenzene			221	U.S. EPA (1994)
Diffusivity in air	D_g^a	cm^2/s		
- benzene			0.0870	U.S. EPA (1994)
- toluene			0.0870	U.S. EPA (1994)
- ethylbenzene			0.0750	U.S. EPA (1994)
Diffusivity in water	D_i^w	cm^2/s		
- benzene			9.80 E-06	U.S. EPA (1994a)
- toluene			8.60 E-06	U.S. EPA (1994a)
- ethylbenzene			8.64 E-06	U.S. EPA (1994a)
Henry's law constant	K_H	Unitless		
- benzene			0.22	U.S. EPA (1994)
- toluene			0.26	U.S. EPA (1994)
- ethylbenzene			0.32	U.S. EPA (1994)
Degradation rate constant	μ	1/day	0	Default to eliminate effects of degradation

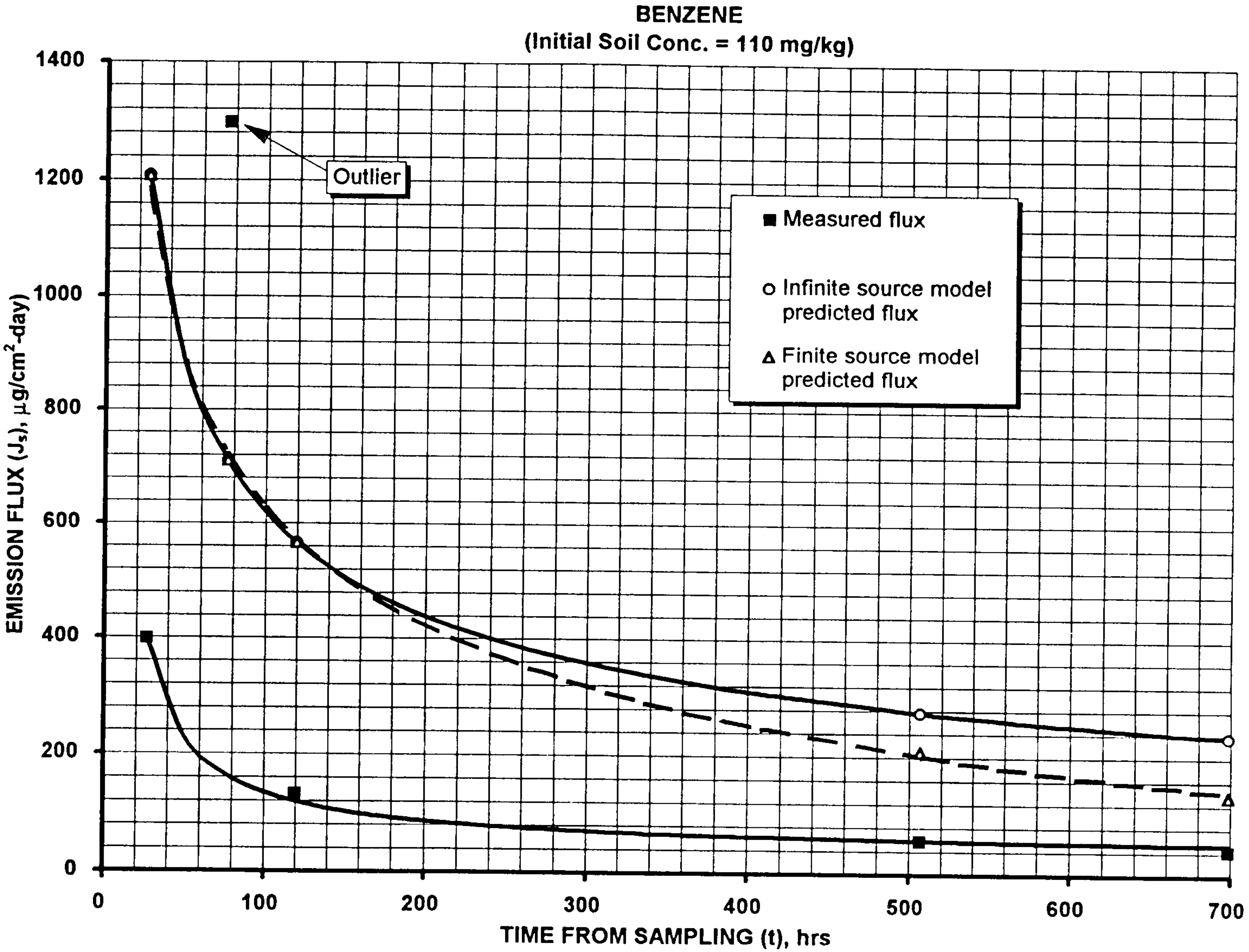


Figure 9
Predicted And Measured Emission Flux Of Benzene (C_o = 110 ppmw)

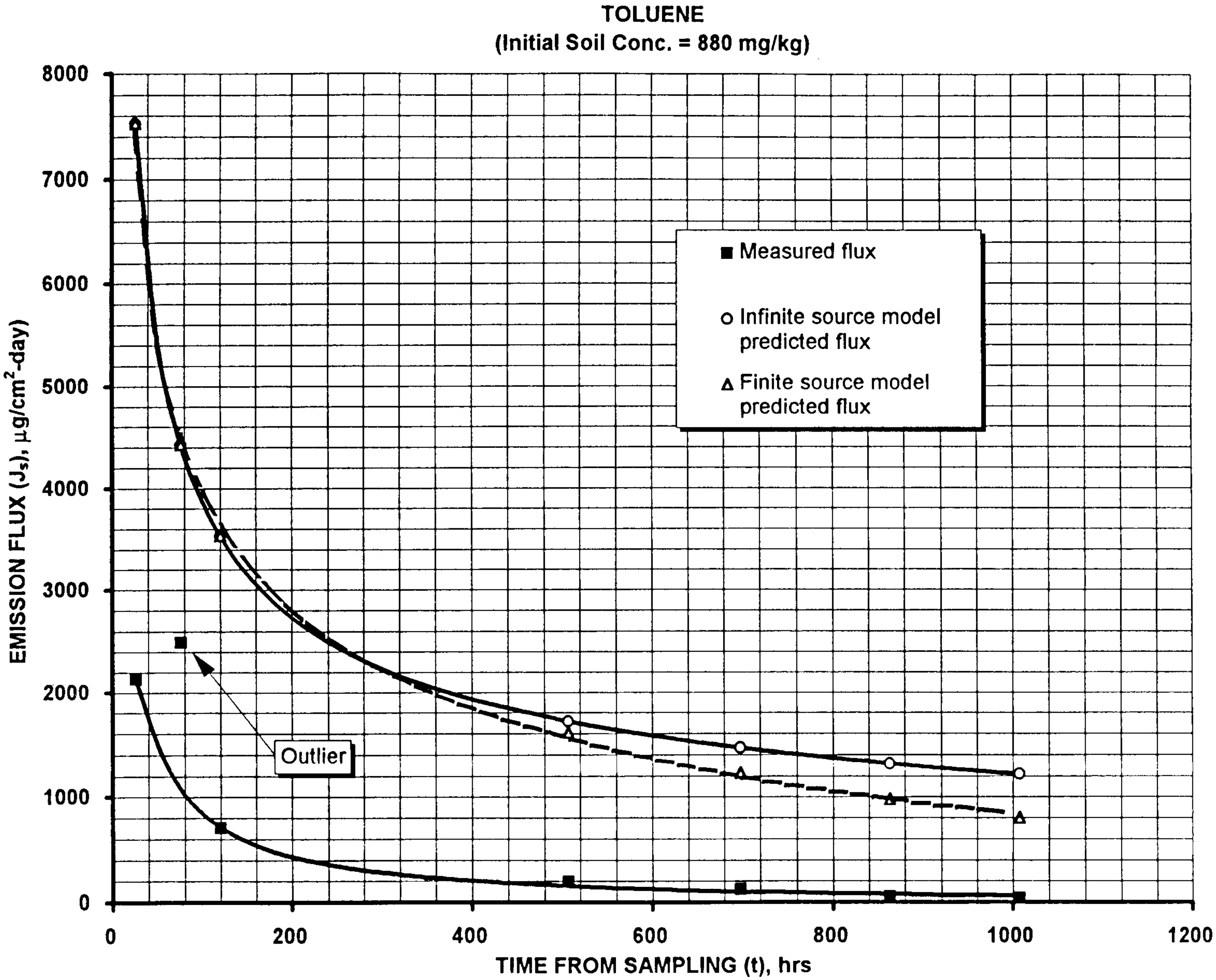


Figure 10
Predicted And Measured Emission Flux Of Toluene (C_o = 880 ppmw)

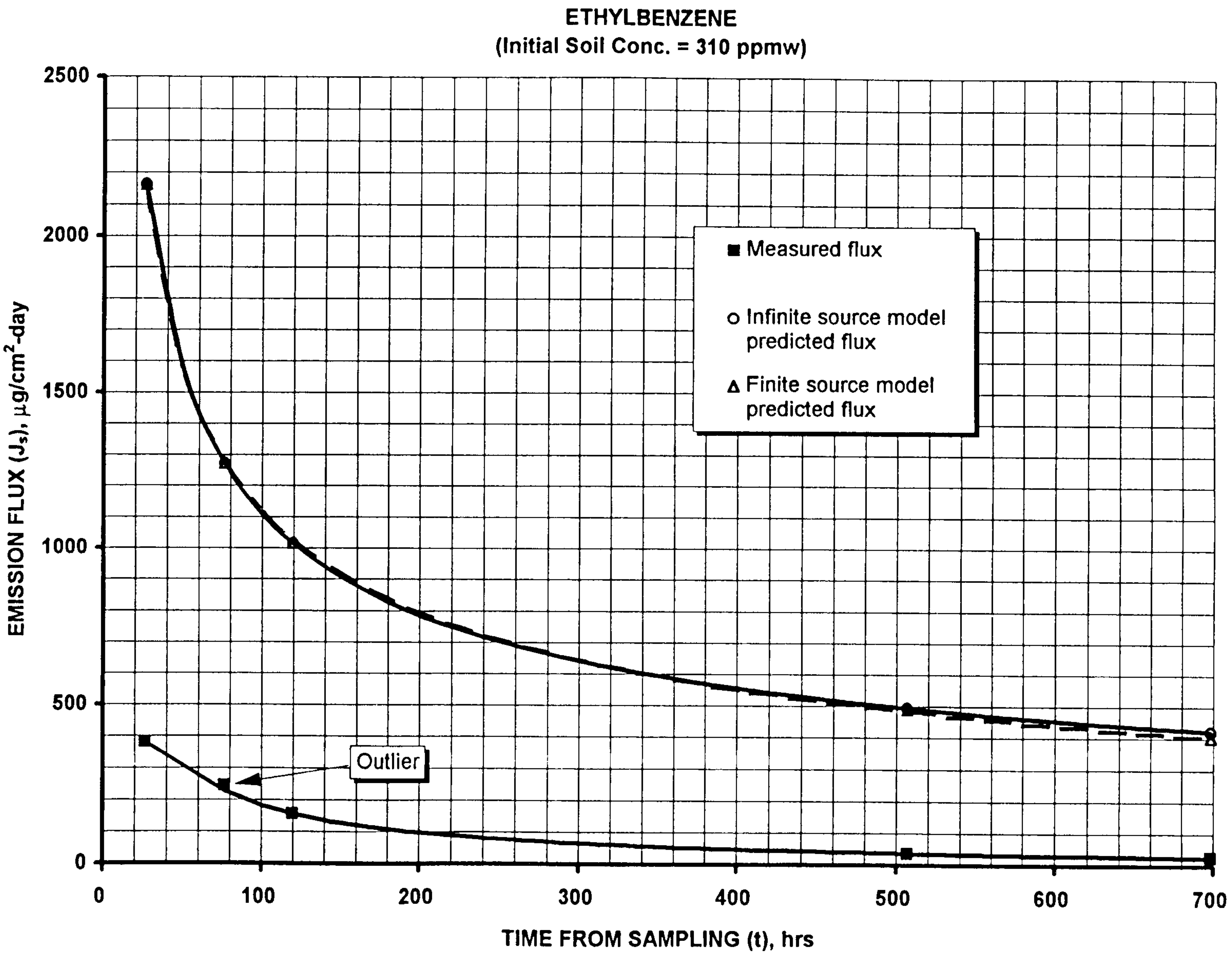


Figure 11
Predicted And Measured Emission Flux Of Ethylbenzene (C_o = 310 ppmw)

TABLE 4.
SUMMARY OF STATISTICAL ANALYSIS OF PILOT-SCALE VALIDATION

Chemical	N	Correlation coefficient	Mean ratio: Modeled-to-measured	p-value	95% confidence interval
Benzene (110 ppm)	5	0.982	2.5	0.0149	(1.4, 4.5)
Toluene (880 ppm)	7	0.988	6.3	0.0002	(3.9, 10.4)
Ethylbenzene (310 ppm)	5	0.999	7.8	0.0008	(4.9, 12.4)

Figures 12, 13, and 14 show the comparison of the log-transformed data for the modeled and measured emission fluxes of benzene, toluene, and ethylbenzene, respectively. As can be seen from Table 4, correlation coefficients ranged from 0.982 for benzene to 0.999 for ethylbenzene, while p-values and 95 percent confidence intervals indicate a significant statistical difference between modeled and measured values.

The boundary conditions of the infinite source model were violated after the first timestep for benzene, and after the third time-step for both toluene and ethylbenzene. The infinite source model predicted 134 percent, 117 percent, and 103 percent of the total mass loss of the finite source model for benzene, toluene, and ethylbenzene, respectively.

In general, the predicted values were higher than the measured values throughout the time-span of the experiment for all three compounds. It is also interesting to note that during the initial stage of the experiment the predicted values were considerably higher than measured values even when contaminant loss at the soil surface due to evaporation was expected. Although the relative differences between predicted and measured values are not excessive (i.e., the highest modeled-to-omeasured mean ratio is within a factor of approximately 10), they are considerably higher than those of the bench-scale studies.

Any one or a combination of the following could account for the larger discrepancies between measured and predicted values in the pilot-scale study:

1. Although the initial soil concentrations of the three compounds were below or within a factor of two of their respective single component saturation concentrations, they may have been greater than the component concentrations for which a residual-phase of gasoline existed. If this were the case, measured emissions may have been in part due to the presence of nonaqueous-phase liquids (NAPL) which would have violated the model's assumptions of equilibrium partitioning.

2. Soil mixing processes and transfer to the test bed may have resulted in heterogenous incorporation of the contaminants. If surface concentrations were reduced due to incomplete mixing, measured emissions would have been reduced during the initial stages of the experiment.

3. Sampling and/or analytical variability may have resulted in under reporting of emission fluxes and/or over reporting of initial soil concentrations.

4. Contaminants sorbed to the test bed liner may have acted to reduce emissions.

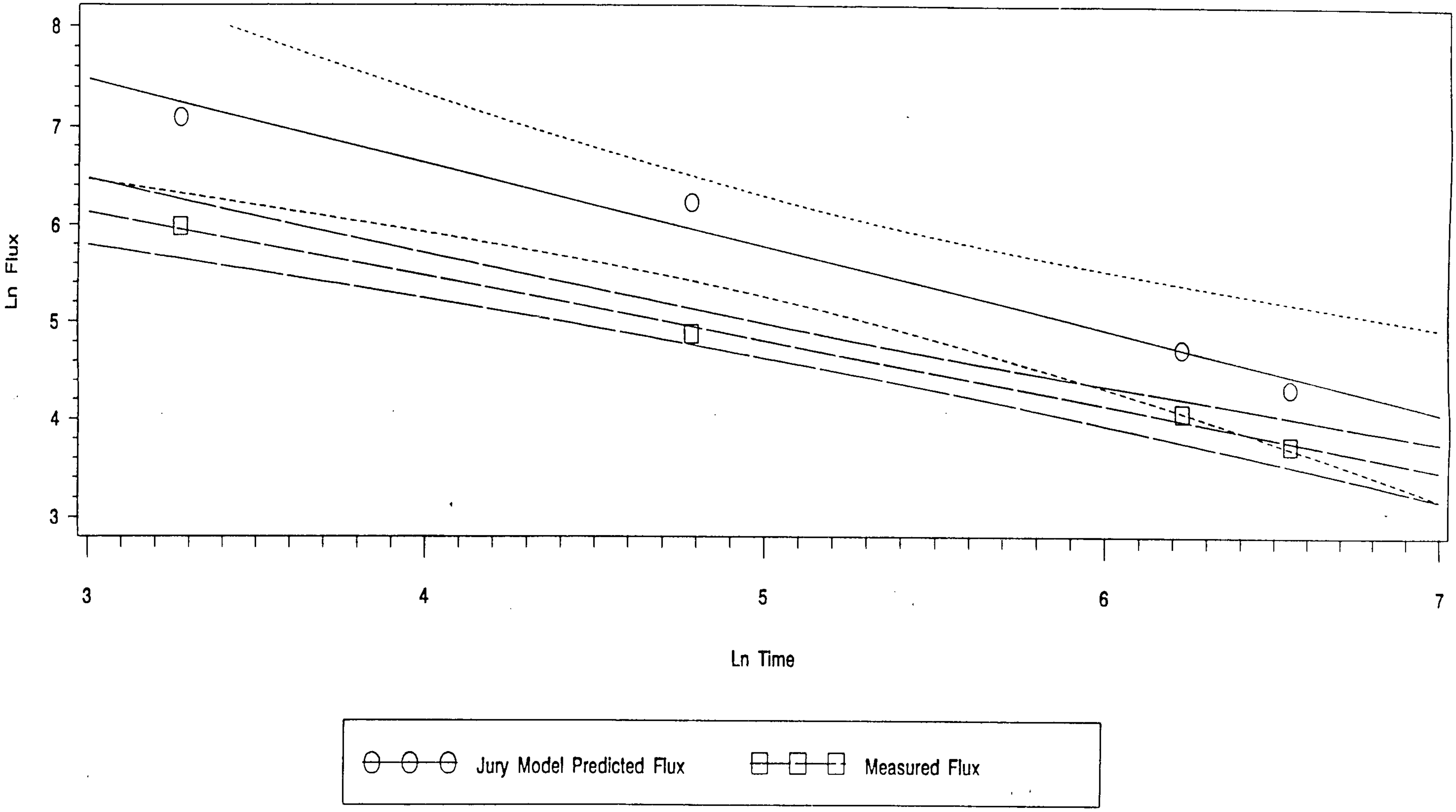


Figure 12
Comparison Of Log-Transformed Modeled And Measured Emission Flux Of Benzene (C_o = 110 ppmw)

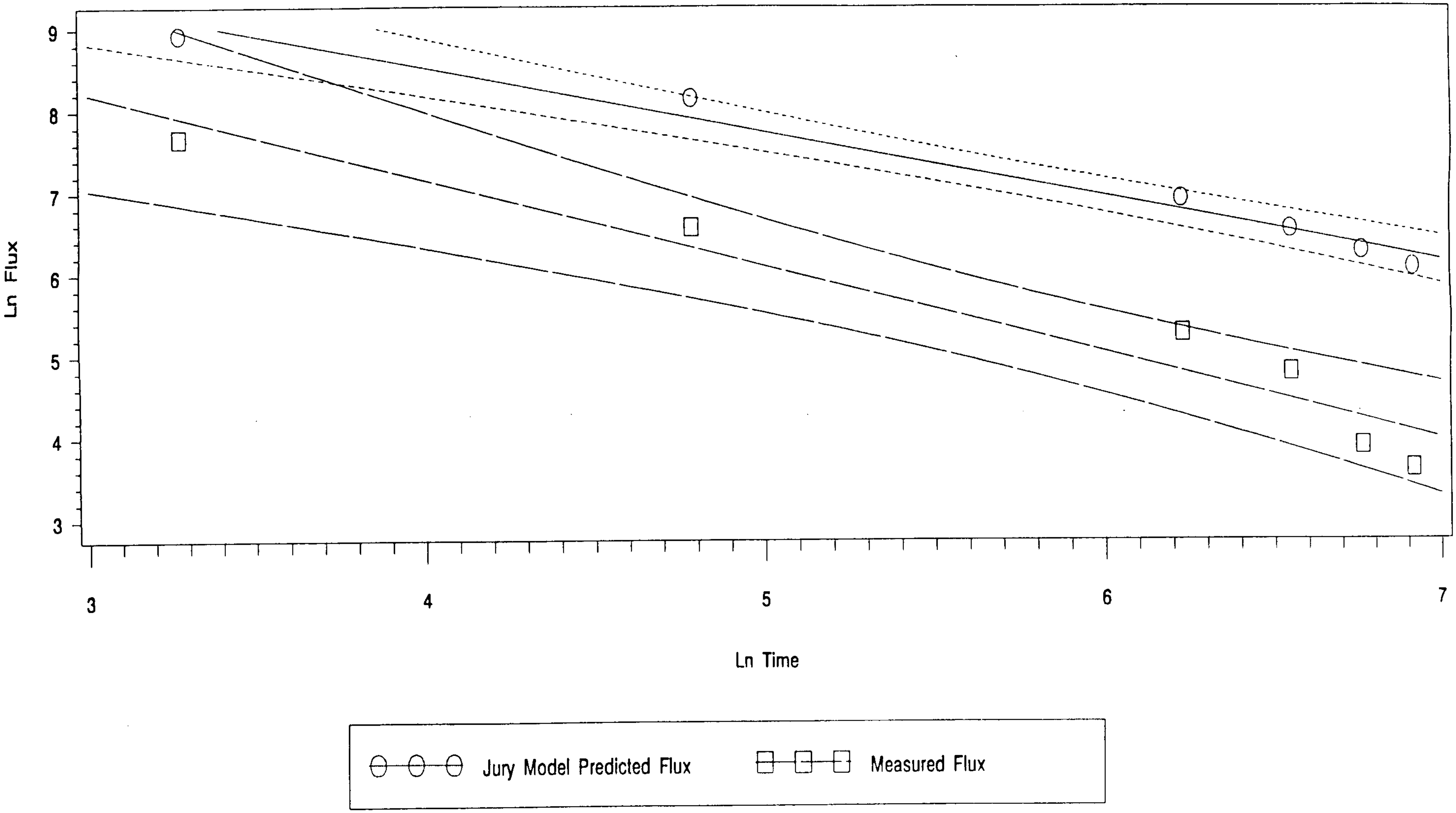


Figure 13
Comparison Of Log-Transformed Modeled And Measured Emission Flux Of Toluene (C_o = 880 ppmw)

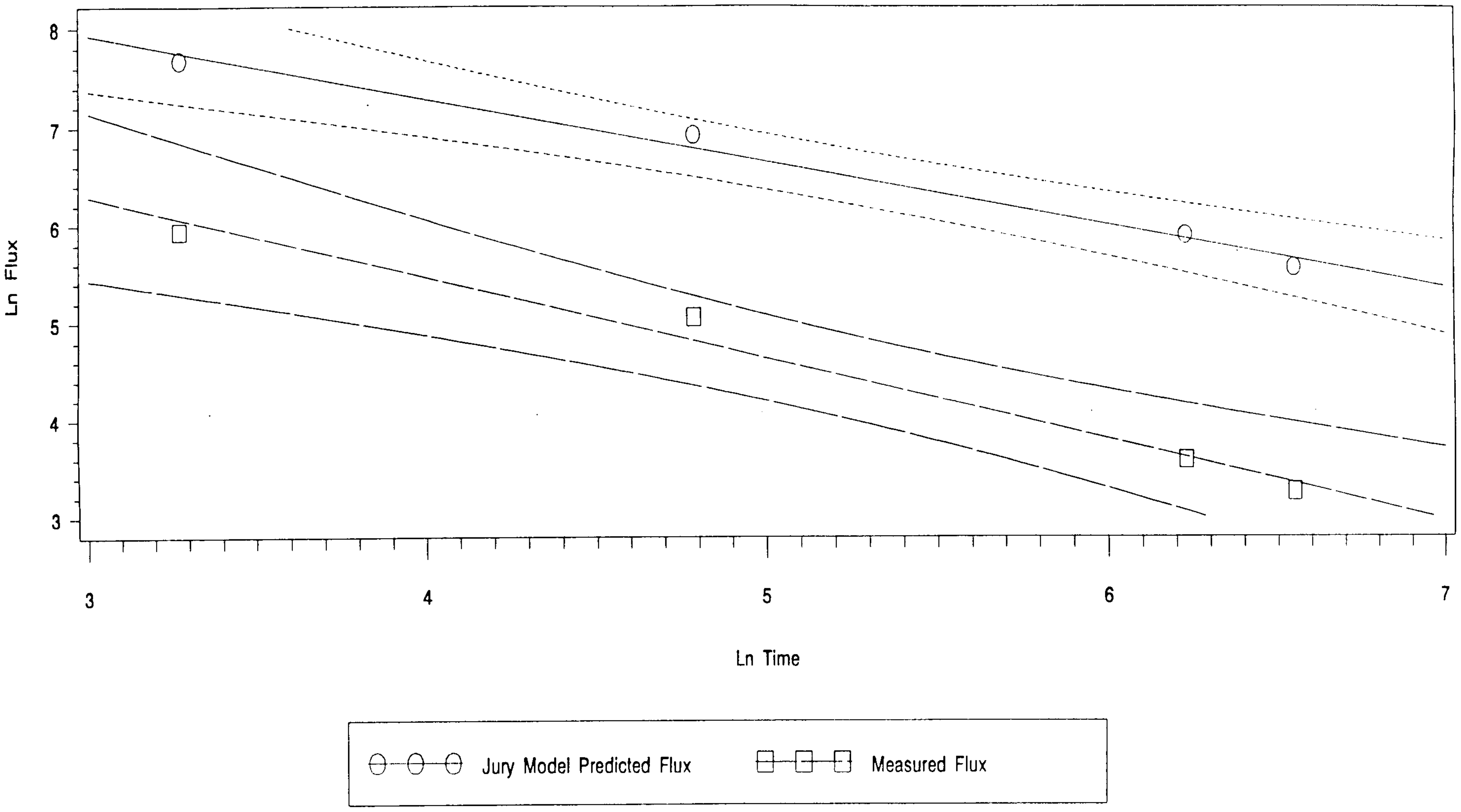


Figure 14
Comparison Of Log-Transformed Modeled And Measured Emission Flux Of Ethylbenzene (C_o = 310 ppmw)

5. Variability in the relative humidity of the air above the test bed may have induced surface water evaporation in between flux chamber samples. Water evaporation would have moved contaminants to the surface by convection and depleted soil concentrations in between sampling events.

6. The model is not as accurate for compounds with relatively high Henry's law constants.

From these observations, it appears more likely that the larger discrepancies between modeled and measured emissions in the pilot-scale study are due to experimental conditions. Sufficient uncertainty exists as to whether all model boundary conditions were maintained during the experiment. For this reason, the results of the pilot-scale validation should be considered less reliable than those of the bench-scale validation. This conclusion suggests that controlled studies should be considered for validation of model predictions for compounds with relatively high Henry's law constants.

3.2 VALIDATION OF THE JURY REDUCED SOLUTION FINITE SOURCE MODEL

From the literature search, one bench-scale study was found that replicated the boundary conditions of the Jury Reduced Solution model (Equation 1). Jury et al. (1980) reports the emissions of the herbicide triallate [S-(2,3,3-trichloroallyl) diisopropyithiocarbamate] incorporated in San Joaquin sandy loam. This study replicated the model boundary conditions in that a clean layer of soil underlayed the contaminated soil allowing diffusion across the lower boundary as well as the upper boundary.

Volatilization of triallate was measured in a closed volatilization chamber (Spencer et al., 1979). The air chamber above the soil was 2 mm deep and 3 cm wide, matching the width of the evaporating surface. An average air flow rate of 1 liter per minute was maintained across the surface equivalent to a windspeed of 1 km/h. Triallate was applied by atomizing the material in hexane onto the air-dry autoclaved soil. The soil was mixed and allowed to equilibrate in a vented fume hood. The soil was then transferred to the chamber and wetted from the bottom. To prevent water evaporation at the soil surface, the chamber was maintained at 100 percent relative humidity and a temperature of 25°C.

The volatilized triallate was trapped daily on polyurethane plugs and extracted and analyzed as described in Grover et al. (1978). The volatilization of triallate at an initial soil concentration of 10 ppmw was measured over a 29 day period in the absence of water evaporation. Calculation of the saturation concentration (C_{sat}) confirmed that the initial concentration of 10 ppmw was in dissolved form. Table 5 gives the values of each variable employed to calculate emissions of triallate using the Jury Reduced Solution volatilization model.

Figure 15 shows the comparison of the predicted and measured values for triallate at an initial soil concentration of 10 ppmw. The data plots indicate very good agreement between modeled and measured values. Figure 16 shows the comparison of the log-transformed data and confidence intervals. From the population of 32 observations, the correlation coefficient was calculated to be 0.998 with a mean modeled-to-measured ratio of 1.11. The p-value was calculated at 0.0001, and the confidence interval was 1.07 to 1.16.

TABLE 5.
VOLATILIZATION MODEL INPUT VALUES FOR TRIALLATE

Variable	Symbol	Units	Value	Reference/Equation
Initial soil concentration	C_o	mg/kg	10	Jury et at. (1980)
Soil depth	L	cm	10	Jury et at. (1980)
Soil dry bulk density	ρ_b	g/cm^3	1.34	Jury et at. (1980)
Soil particle density	ρ_s	g/cm^3	2.65	U.S. EPA (1988)
Gravimetric soil moisture content	w	percent	21	Calculated from Jury et al. (1980)
Water-filled soil porosoty	Θ	cm^3/cm^3	0.279	Jury et at. (1980)
Total soil porosity	ϕ	cm^3/cm^3	0.494	Jury et at. (1980)
Air-filled soil porosity	a	cm^3/cm^3	0.215	Jury et at. (1980)
Soil organic carbon	f_{oc}	fraction	0.0072	Calculated from Jury et al. (1980)
Organic carbon partition coefficient	K_{oc}	cm^3/g	3600	Jury et at. (1980)
Diffusivity in air	D_g^a	cm^2/d	3888	Jury et at. (1980)
Diffusivity in water	D_i^w	cm^2/d	0.432	Jury et at. (1980)
Henry's law constant	K_H	unitless	1.04 E-03	Jury et at. (1980)
Degradation rate constant	μ	1/day	0	Default to eliminate effects of degradation

The degree of agreement between modeled and measured emission flux values for triallate may be due to soil adsorption studies conducted to experimentally derive the organic carbon partition coefficient specific to the San Joaquin sandy loam used in the experiment. With experimentally derived values of K_{oc}, more accurate phase partitioning was possible resulting in an experimental-specific value of the effective diffusion coefficient (Equation 2). Appendix B contains the spreadsheet calculations for the bench-scale validation of the Jury Reduced Solution finite source volatilization model.

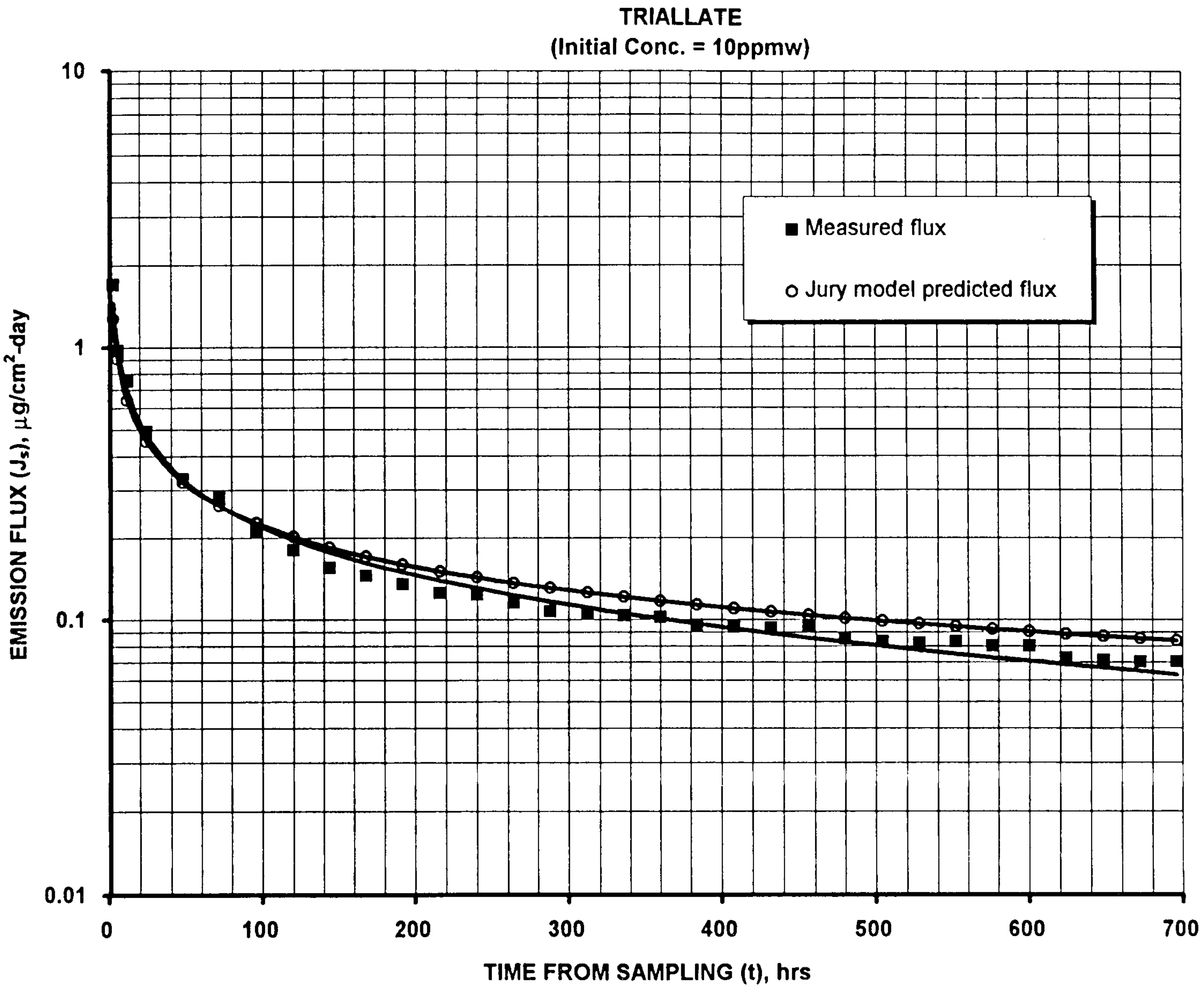


Figure 15
Predicted And Measured Emission Flux Of Triallate Versus Time

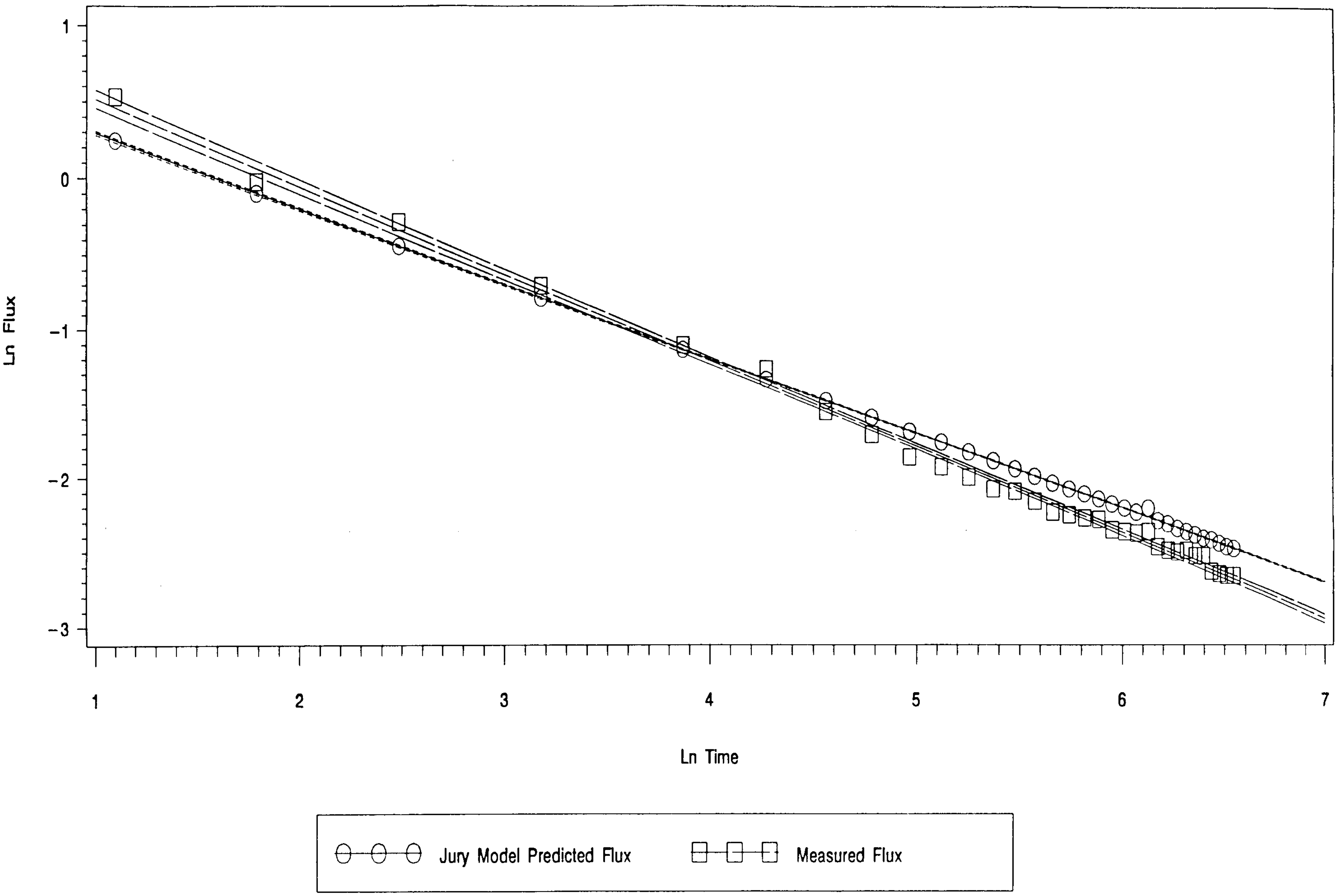


Figure 16
Comparison Of Log-Transformed Modeled And Measured Emission Flux Of Triallate

SECTION 4

PARAMETRIC ANALYSIS OF THE JURY VOLATILIZATION MODELS

This section presents the results of parametric analysis of the key variables of the Jury volatilization models (Equations 1 and 3). The Jury volatilization models are applicable for the case of no boundary layer resistance at the soil-air interface and no water flux through the soil column. Because the models are equivalent to the Mayer et al. (1974) solutions to the general diffusion equation (Equation 5), the parametric observations of Mayer et al. (1974) and Farmer, et al. (1980) are also directly applicable.

Jury et al. (1983) established the relationship between vapor and solute diffusion and adsorption by defining total phase concentration partitioning as it relates to the effective diffusion coefficient. The effective diffusion coefficient is a theoretical expression of the combination of soil parameters and chemical properties which govern the rate at which soil contaminants move to the surface to replace those lost by evaporation. As such, the effective diffusion coefficient is the rate-limiting factor governing the general diffusion equation in soils given the initial and boundary conditions for which the models are applicable. The remainder of this section discusses the key soil and nonsoil parameters used in the expression of the effective diffusion coefficient and the general diffusion equation.

4.1 AFFECTS OF SOIL PARAMETERS

In this section, the experimental results of Farmer, et al. (1980) are discussed as they relate to the effect of soil water content, soil bulk density, air-filled soil porosity, and temperature on diffusion in soil.

Soil Moisture Content

Farmer, et al. (1980) indicates that the effect of soil moisture content on the volatilization flux of contaminants through soils is exponential. Increasing soil water content decreases the pore spaces available for vapor diffusion and will decrease volatilization flux. In contrast, increasing soil water content has also been shown to increase the volatility of pesticides in soil under certain conditions (Gray, et al., 1965; and Spencer and Cliath, 1969 and 1970). In essence, the soil water content affects the contaminant adsorption capacity by competing for soil adsorption sites. Under these conditions, an increase in soil moisture above a certain point will tend to desorb contaminants, increasing the flux dependent on the relative water and contaminant adsorption isotherms.

Bulk Density

Soil compaction or bulk density also determines the porosity of soil and thus affects the diffusion through the soil. Experimental results from Farmer et al. (1980) indicate that soil bulk density also has an exponential effect on volatilization flux through the soil. From previous considerations of the effect of soil water content, a higher bulk density will have similar effects to that of an increased soil moisture content.

Soil Air-Filled Porosity

The effects of soil water content and soil bulk density on volatilization can be contributed to their effect on the air-filled porosity, which in turn is the major soil factor controlling volatilization. The effect of air-filled porosity is manifested in the expression of the effective diffusion coefficient. The effective diffusion coefficient, however, does not depend only on the amount of air-filled pore space. The presence of liquid film on the solid surfaces not only reduces porosity, but also modifies the pore geometry increasing tortuosity and the length of the gas passage. The Jury et al. (1983) expression of the effective diffusion coefficient uses the model of Millington and Quirk (1961) to account for the porosity and the tortuosity of soil as a porous medium.

Soil Temperature

The effect of soil temperature on the volatilization flux is multifunctional. The diffusion in air, D_g^a, is theoretically related to temperature, T, and the collision integral, Ω, in the following manner (Lyman, et al., 1990):

$$D_g^a \text{ (proportional to) } \frac{T^{0.5}}{\Omega(T)} \tag{15}$$

The exponential coefficient for temperature varies from 1.5 to 2 over a wide range of temperatures. Barr and Watts (1972) found that 1.75 gave the best values for gaseous diffusion. Farmer, et al. (1980) estimates the effective diffusion coefficient at temperature T_2 as:

$$D_2 = D_1 \, (T_2 / T_1)^{0.5} \tag{16}$$

where D_2 = Diffusion coefficient at T_2

D_1 = Diffusion coefficient at T_1

T = Absolute temperature.

A temperature increase will effect the vapor pressure function of the Henry's Law constant, which causes an increase in the vapor concentration gradient across the soil layer. In actual fact, temperature gradients will exist across the soil due primarily to seasonal variations. Vapor diffusion is influenced by such gradients; however, these effects of fluctuating soil temperatures will tend to cancel one another over time.

4.2 AFFECTS OF NONSOIL PARAMETERS

The nonsoil variables in the Jury volatilization models include the initial soil concentration, C_o, the Henry's law constant (K_H), the soil/water partition coefficient, (K_D) and the depth of contaminant incorporation (L).

Initial Soil Concentration

The effect of change in the initial soil concentration is linear; i.e., an increase in C_o of 100 percent causes an increase in the emission rate of 100 percent. Probably the greatest degree of uncertainty in the value of C_o is likely to be either insufficient soil sampling to adequately characterize site soil concentrations, or the variability in percent recovery of contaminants as it applies to existing sampling and analysis methods for organic compounds in soils. Typically, present extraction and analysis method recovery variability increases the likelihood of underprediction of the emission rate (i.e., more contaminant is present in the soil than is reported by sampling and analysis methods).

Henry's Law Constant and Soil/Water Partition Coefficient

Jury et al. (1984) showed that a given chemical can be grouped into three main categories depending on the ratio K_D/K_H. These categories are defined as a function of which phase dominates diffusion. A Category I chemical is dominated by the vapor-phase, a Category III chemical by the liquid-phase, and Category II chemicals by vapor-phase diffusion at low soil water content and liquid-dominated at high water content. Desorption from the solid-phase to the liquid-phase is a function of the soil/water partition coefficient, while volatilization from the liquid to the vapor-phase is a function of the Henry's law constant. Therefore, the interstitial vapor density, and thus emission flux, is directly proportional to K_H and inversely proportional to K_D. Because the Jury volatilization models do not account for a soil-air boundary layer, the effects of K_H and K_D are exponential for all three categories of chemicals.

Depth of Contaminant Incorporation

The Jury Reduced Solution finite source model accounts for diffusion across both the upper and lower boundaries. Therefore for chemicals with high effective diffusion coefficients, the residual soil concentration will decrease rapidly. In this regard, the emission flux curve will become asymptotic more rapidly than for the semi-infinite case (Equation 3). The exponential term $[1 - \exp(-L^2/4\ D_E t)]$ in Equation 1 accounts for diffusion across the lower boundary such that the term decreases rapidly with time for small values of L and large values of D_E.

SECTION 5

CONCLUSIONS

From the results of this study, it can be concluded that for the compounds included in the experimental data, both models showed good agreement with measured data given the conditions of each test. Each model demonstrated superior agreement with bench-scale measured values and to a lesser extent the infinite source model with pilot-scale data. The results indicate high correlation coefficients across all experimental data with mean modeled-to-measured ratios as low as 0.37 and as high as 7.8.

From a review of test conditions, it was concluded that the bench-scale studies better approximated the initial and boundary conditions of the infinite source model. This is evident in the lower modeled-to-measured mean ratios and narrow 95 percent confidence intervals. Although the pilot-scale study data showed reasonable agreement with predicted values, questions remain as to whether the test conditions were in agreement with model assumptions and accurately replicated all model boundary conditions. Overall, each model provided reasonably accurate predictions.

Clearly, this validation study is limited by the range of conditions simulated, the assumptions under which the models operate, and the initial and boundary conditions of each model. Important limitations include:

1. The duration of the experiments examined range from 7 to 36 days. Model performance for longer periods could not be validated.

2. Both models assume no mass flow of contaminants due to water movement in the soil. Mass flow due to capillary action or redistribution of contaminates due to rain events may be significant if applicable to site-specific condition.

3. The models are valid only if the effective diffusion coefficient in soil is constant. This assumes isotropic soils and completely homogeneous incorporation of contaminants. In reality, soils are usually heterogeneous, with properties that change with depth (e.g., fraction of organic carbon, water content, porosity, etc.). The user will need to carefully consider the characterization of soil properties before assigning model input parameters.

4. The equilibrium partitioning relationships used in the models are no longer valid for pure-phase chemicals or when high dissolved concentrations are present. Therefore, the models should not be used when these conditions exist.

5. The models do not consider the effects of a soil-air boundary layer on the volatilization rate. For chemicals with Henry's law constants less than approximately 2.5×10^{-5}, volatilization is highly dependent on the thickness of the boundary layer (Jury et al., 1984). A boundary layer will restrict volatilization if the maximum flux through the boundary layer is small compared to the rate at which the contaminant moves to the surface. In this case, the volatilization rate is inversely proportional to the boundary layer thickness.

6. In the case of the infinite source model, validation for chemicals with relatively high Henry's law constants requires that the depth of contamination be sufficient to prevent loss at the lower boundary over the duration of the experiment, i.e., $L > (18.4\ D_E\ t)^{1/2}$. Although this study indicates that the Jury Infinite Source model exhibited a relatively small maximum error (i.e., 134% of the Mayer et al. finite source model total mass loss for benzene), any future validation studies should

maintain a sufficient depth of incorporation to prevent violation of the model boundary conditions.

7. No experimental data could be found in the literature for validation of the Jury Reduced solution finite source model for compounds with high Henry's law constants.

Emission rates predicted by the Jury Infinite Source volatilization model and the Jury Reduced Solution finite source volatilization model indicate good correlation to measured emission rates under controlled conditions, but predicted values for field conditions would be subject to error because the boundary conditions and environmental conditions are not as well defined as they are in the laboratory. Nonetheless, results of this study indicate that both models should make reasonable estimates of loss through volatilization at the soil surface given the boundary conditions of each model.

REFERENCES

Balfour, W. D., B. M. Eklund, and S. J. Williamson. Measurement of Volatile Organic Emissions from Subsurface Contaminants. In *Proceedings of* the *National Conference on Management of Uncontrolled Hazardous Waste Sites*. September 1984, pp. 77-81. Hazardous Materials Control Research Institute, Silver-Springs, Maryland.

Barr, R. F. and H. F. Watts. 1972. Diffusion of Some Organic and Inorganic Compounds in Air. J. Chem. *Eng. Data* 17:45-46.

Carslaw, H. S., and J. C. Jaeger. 1959. *Conduction of Heat in Solids.* zd Edition Oxford University Press, Oxford.

Environmental Quality Management, Inc. 1994. *A Comparison of Soil Volatilization Models in Support of Superfund Soil Screening Level Development. U.S.* Environmental Protection Agency, Contract No. 68-D30035, Work Assignment No. 0-25.

Farmer, W. J., K. Igue, W. F. Spencer, and J. P. Martin. 1972. Volatility of Organochlorine Insecticides from Soil. I and II Effects. *Soil Sci. Soc. Amer. Proc.* 36:443-450.

Farmer, W. J., and J. Letey. 1974. *Volatilization Losses of Pesticides From Soils.* Office of Research and Development. EPA-660/2-74/054.

Farmer, W. J., M. S. Yang, J. Letey, and W. F. Spencer. 1980. *Land Disposal of Hexachlorobenzene Wastes.* Office of Research and Development. EPA-600/2-80/119.

Gray, R. A., and A. J. Weierch. 1965. Factors Affecting the Vapor Loss of EPTC from Soil. *Weeds* 13:141-147.

Grover, R., W. F. Spencer, W. J. Farmer, and T. D. Shoup. 1978. Triallate Vapor Pressure and Volatilization from Glass Surfaces. *Weed Sci.,* 26:505-508.

Hill, F. B., V. P. Aneja, and R. M. Felder. 1978. A Technique for Measurement of Biogenic Sulfur Emission Fluxes. *J. Env. Sci. Health* AIB (3), pp. 199-225.

Howard, P. H., R. S. Boethling, W. F. Jarvis, W. M. Meylan, and E. O. Michaelenko. 1991. *Handbook* of *Environmental Degradation Rates.* Lewis Publishers, Chelsea, Michigan.

Jury, W. A., R. Grover, W. F. Spencer, and W. J. Farmer. 1980. Modeling Vapor Losses of Soil-lncorporated Triallate. *Soil Science Society Am. J.,* 44:445-450.

Jury, W. A., W. F. Spencer, and W. J. Farmer. 1983. Behavior Assessment Model of Trace Organics in Soil: I. Model Description. *J. Environ. Qual.,* Vol. 12, No. 4:558:564.

Jury, W. A., W. J. Farmer, and W. F. Spencer. 1984. Behavior Assessment Model for Trace Organics in Soil: II. Chemical Classification and Parameter Sensitivity. *J. Environ. Qual.,* Vol. 13, No. 4:567-572.

Jury, W. A., D. Russo, G. Streile, and H. El Abd. 1990. Evaluation of Volatilization by Organic Chemicals Residing Below the Soil Surface. *Water Resources Res.,* Vol. 26, No. 1:13-20.

Kienbusch, M. *Measurement* of *Gaseous Emission Rates from Land Surfaces Using an Emission Isolation Flux Chamber - User's Guide*. Report to EPA-EMSL, Las Vegas under EPA Contract No. 68-02-3889, Work Assignment No. 18, December 1985.

Kienbusch, M. and D. Ranum. 1986. *Validation of Flux Chamber Emission Measurements on Soil Surface* - Draft Report to EPA-EMSL, Las Vegas, Nevada.

Kienbusch, M., W. D. Balfour, and S. Williamson. *The Development of an Operations Protocol for Emission Isolation Flux Chamber Measurements on Soil Surfaces.* Presented at the 79th Annual Meeting of the Air Pollution Control Association (Paper 86-20.1), Minneapolis, Minnesota, June 22-27, 1986.

Lyman, W. J., W. F. Reehl, and D. H. Rosenblatt. 1990. *Handbook* of *Chemical Property Estimation Methods.* American Chemical Society, Washington, D.C.

Millington, R. J., and J. M. Quirk. 1961. Permeability of Porous Solids. *Trans. Faraday* Soc. 57:1200-1207.

Radian Corporation. *Soil Gas Sampling Techniques* of *Chemicals* for *Exposure Assessment - Data Volume.* Report to EPA-EMSL, Las Vegas under EPA Contract No. 68-02-3513, Work Assignment No. 32, March 1984.

Radian Corporation. *Short-term Fate and Persistence* of *Motor Fuels in Soils.* Report to the American Petroleum Institute, Washington, D.C. July 1989.

Spencer, W. F., M. Cliath, and W. J. Farmer. 1969. Vapor Density of Soil Applied HEOD as Related to Soil Water Content, Temperature, and HEOD Concentration. *Soil Sci. Soc. Amer. Proc.* 33:509-511.

Spencer, W. F., and M. Cliath. 1970. Vapor Density and Apparent Vapor Pressure of Lindane (γ-BHC). *J. Agr. Food Chem. 18*:529-530.

Spencer, W. F., T. D. Shoup, M. M. Cliath, W. J. Farmer, and R. Haque. 1979. Vapor Pressures and Relative Volatility of Ethyl and Methyl Parathion. *J. Agric. Food Chem.,* 27:273-278.

Spencer, W. F. 1970. Distribution of Pesticides Between Soil, Water and Air. In *Pesticides in the Soil: Ecology, Degradation and Movement.* A symposium, February 25-27, 1970. Michigan State University.

U.S. Environmental Protection Agency. 1988. *Superfund Exposure Assessment Manual.* Office of Emergency and Remedial Response. EPA-540/1-88-001.

U.S. Environmental Protection Agency. 1990. *Procedures for Conducting Air Pathway Analyses for Superfund Activities, Interim Final Documents: Volume 2 - Estimation of Baseline Air Emissions at Superfund Sites.* Office of Air Quality Planning and Standards. EPA-450/1-89-002a.

U.S. Environmental Protection Agency. 1991. *Risk Assessment Guidance for Superfund, Volume 1, Human Health Evaluation Manual (Part B).* Office of Emergency and Remedial Response. Publication No. 9285.7-01B.

U.S. Environmental Protection Agency. 1991a. *Database of Emission Rate Measurement Projects - Technical Note.* Office of Air Quality Planning and Standards. EPA-450/1 -91 003.

U.S. Environmental Protection Agency. 1994. *Technical Background Document for Soil Screening Guidance - Review Draft.* Office of Solid Waste and Emergency Response. EPA-540/R-94/102.

U.S. Environmental Protection Agency. 1994a. *CHEMDAT8 Data Base of Compound Chemical and Physical Properties.* Office of Air Quality Planning and Standards Technology Transfer Network, CHIEF Bulletin Board. Research Triangle Park, North Carolina.

APPENDIX A

VALIDATION DATA FOR THE JURY INFINITE SOURCE MODEL

DIELDRIN 5 PPM
(1 of 2)

Chemical	Sample Point	Initial soil conc.,	Initial soil conc.,	Emitting area	Soil Depth	Soil Type	Soil bulk density,	Soil particle density,	Gravimetric soil moisture,	Water-filled soil porosity,	Solubility	Soil organic carbon,	Saturation conc.,	C_o>C_{sat}	Measured emission flux	Organic carbon part. coeff.,
		C_o	C_o		(L)		ρ_b	ρ_s	w	Θ	S	f_{oc}	C_{sat}		(μg/m^2-	K_{oc}
		(mg/kg)	(g/g)	(cm^2)	(cm)		Kg/L	Kg/L	(wt. fraction)	(unitless)	(mg/L)	(fraction)	(mg/kg)	(Yes/No)	min)	(cm^3/g)
Dieldrin	1	5	5.00E-06	27.55	0.5	GilaSlit Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	200	10900
Dieldrin	2	5	5.00E-06	27.55	0.5	Gila Slit Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	115	10900
Dieldrin	3	5	5.00E-06	27.55	0.5	Gila Slit Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	75	10900
Dieldrin	4	5	5.00E-06	27.55	0.5	Gila Slit Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	65	10900
Dieldrin	5	5	5.00E-06	27.55	0.5	Gila Slit Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	60	10900
Dieldrin	6	5	5.00E-06	27.55	0.5	Gila Slit Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	55	10900
Dieldrin	7	5	5.00E-06	27.55	0.5	Gila Slit Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	40	10900

DIELDRIN 5 PPM
(2 of 2)

Chemical	Soil/water part. coeff.,	Diffusivity in air,	Diffusivity in water,	Effective diffusion coefficient,	Henry's law constant,	Total soil porosity,	Air-filled soil porosity,	Measured emission flux emission flux	Time, t	$t > L^2/14.4\ D_E$	Infinite source model emission flux
	K_D	$D_g{}^a$	$D_i{}^w$	D_E	K_H	ϕ	a		Cumulative		
	(cm^3/g)	(cm^2/s)	(cm^2/s)	(cm^2/s)	(unitless)	(unitless)	(unitless)	($\mu g/cm^2$-day)	(hours)	(Yes/No)	($\mu g/cm^2$-day)
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.2000	24	No	0.0714
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.1150	72	No	0.0412
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.0750	120	No	0.0319
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.0650	144	No	0.0292
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.0600	168	No	0.0270
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.0550	216	No	0.0238
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.0400	288	No	0.0206

DIELDRIN 10 PPM
(1 of 2)

Chemical	Sample Point	Initial soil conc.,	Initial soil conc.,	Emitting area	Soil Depth	Soil Type	Soil bulk density,	Soil particle density,	Gravimetric soil moisture,	Water-filled soil porosity,	Solubility,	Soil organic carbon,	Saturation conc.,	$C_o>C_{sat}$	Measured emission flux	Organic carbon part. coeff.,
		C_o	C_o		(L)		ρ_b	ρ_s	w	Θ	S	f_{oc}	C_{sat}		(ng/cm^2	K_{oc}
		(mg/kg)	(g/g)	(cm^2)	(cm)		(g/cm^3)	(g/cm^3)	(wt. fraction)	(unitless)	(mg/L)	(fraction)	(mg/kg)	(Yes/No)	-day)	(cm^3/g)
Dieldrin	1	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	0 1870	0.0058	12	No	400	10900
Dieldrin	2	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	260	10900
Dieldrin	3	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	140	10900
Dieldrin	4	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	110	10900
Dieldrin	5	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	105	10900
Dieldrin	6	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	0 1870	0.0058	12	No	90	10900
Dieldrin	7	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	0.1870	0.0058	12	No	85	10900

DIELDRIN 10 PPM
(2 of 2)

Chemical	Soil/ water part. coeff.,	Diffusivity in air,	Diffusivity in water,	Effective diffusion coefficient,	Henry's law constant,	Total soil porosity,	Air-filled soil porosity,	Measured emission flux	Time, t	$t > L^2/14.4\ D_E$	Infinite source model emission flux
	K_D	D_g^a	D_i^w	D_E	K_H	ϕ	a		Cumulative		
	(cm^3/g)	(cm^2/s)	(cm^2/s)	(cm^2/s)	(unitless)	(unitless)	(unitless)	($\mu g/cm^2$-day)	(hrs)	(Yes/No)	($\mu g/cm^2$-day)
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.4000	24	No	0.1428
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.2600	72	No	0.0825
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.1400	120	No	0.0639
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.1100	144	No	0.0583
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.1050	168	No	0.0540
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.0900	216	No	0.0476
Dieldrin	63.22	0.0125	4.74E-06	1.32E-08	0.00011	0.7170	0.6420	0.0850	288	No	0.0412

LINDANE 5 PPM
(1 of 2)

Chemical	Sample Point	Initial soil conc.	Initial soil conc.	Emitting area	Soil Depth	Soil Type	Soil bulk density,	Soil particle density,	Gravimetric soil moisture,	Water-filled soil porosity,	Solubility,	Soil organic carbon,	Saturation conc.,	$C_o > C_{sat}$	Measured emission flux	Organic carbon part. coeff.,
		C_o	C_o		(L)		ρ_b	ρ_s	w	Θ	S	f_{oc}	C_{sat}			K_{oc}
		(mg/kg)	(g/g)	(cm^2)	(cm)		(g/cm^3)	(g/cm^3)	(wt. fraction)	(unitless)	(mg/L)	(fraction)	(mg/kg)	(Yes/No)	(ng/cm^2-day)	(cm^3/g)
Lindane	1	5	5.00E-06	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	4.2000	0.0058	34	No	500	1380
Lindane	2	5	5.00E-06	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	4.2000	0.0058	34	No	160	1380
Lindane	3	5	5.00E-06	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	4.2000	0.0058	34	No	60	1380
Lindane	4	5	5.00E-06	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	4.2000	0.0058	34	No	40	1380

LINDANE 5 PPM
(2 of 2)

Chemical	Soil/water part. coeff.,	Diffusivity in air,	Diffusivity in water,	Effective diffusion coefficient,	Henry's law constant,	Total soil porosity,	Air-filled soil porosity,	Measured emission flux	Time, t	$t > L^2/14.4\ D_E$	Infinite source model emission flux	Finite source model emmision flux	Infinite source model error
	K_D	D_g^a	D_l^w	D_E	K_H	ϕ	a		Cumulative				
	(cm^3/g)	(cm^2/s)	(cm^2/s)	(cm^2/s)	(unitless)	(unitless)	(unitless)	($\mu g/cm^{2-}$day)	(hours)	(Yes/No)	($\mu g/cm^{2-}$day)	($\mu g/cm^{2-}$day)	(percent)
Lindane	8.00	0.0176	5.57E-06	1.80E-07	0.00014	0.7170	0.6420	0.5000	24	No	0.2641	0.2641	0.0000
Lindane	8.00	0.0176	5.57E-06	1.80E-07	0.00014	0.7170	0.6420	0.1600	72	Yes	0.1525	0.1510	0.9604
Lindane	8.00	0.0176	5.57E-06	1.80E-07	0.00014	0.7170	0.6420	0.0600	120	Yes	0.1181	0.1086	8.7891
Lindane	8.00	0.0176	5.57E-06	1.80E-07	0.00014	0.7170	0.6420	0.0400	168	Yes	0.0998	0.0797	25.2965

LINDANE 10 PPM
(1 OF 2)

Chemical	Sample Point	Initial soil conc.,	Initial soil conc.,	Emitting area	Soil Depth	Soil Type	Soil bulk density,	Soil particle density,	Gravimetric soil moisture,	Water-filled soil porosity,	Solubility,	Soil organic carbon,	Saturation conc.,	$C_o > C_{sat}$	Measured emission flux	Organic carbon part. coeff.,
		C_o	C_o		(L)		ρ_b	ρ_s	w	Θ	S	f_{oc}	C_{sat}		(ng/cm^2	K_{oc}
		(mg/kg)	(g/g)	(cm^2)	(cm)		(g/cm^3)	(g/cm^3)	(wt. fraction)	(unitless)	(mg/L)	(fraction)	(mg/kg)	(Yes/No)	-day)	(cm^3/g)
Lindane	1	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	4.2000	0.0058	34	No	1160	1380
Lindane	2	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	4.2000	0.0058	34	No	320	1380
Lindane	3	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	4.2000	0.0058	34	No	140	1380
Lindane	4	10	1.00E-05	27.55	0.5	Gila Silt Loam	0.75	2.65	0.10	0.0750	4.2000	0.0058	34	No	90	1380

LINDANE 10 PPM
(2 of 2)

Chemical	Soil/water part. coeff.,	Diffusivity in air,	Diffusivity in water,	Effective diffusion coefficient,	Henry's law constant,	Total soil porosity,	Air-filled soil porosity,	Measured emission flux	Time, t	$t > L^2/14.4\ D_E$	Infinite source model emission flux	Finite source model emmision	Infinite source model error
	K_D	D_g^a	D_i^w	D_E	K_H	ϕ	a	(μg/cm^2	Cumulative		(μg/cm^2	(μg/cm^2	
	(cm^3/g)	(cm^2/s)	(cm^2/s)	(cm^2/s)	(unitless)	(unitless)	(unitless)	-day)	(hours)	(Yes/No)	-day)	-day)	(percent)
Lindane	8.00	0.0176	5.57E-.06	1.80E-07	0.00014	0.7170	0.6420	1.1600	24	No	0.5282	0.5282	0.0000
Lindane	8.00	0.0176	5.57E-.06	1.80E-07	0.00014	0.7170	0.6420	0.3200	72	Yes	0.3049	0.3020	0.9604
Lindane	8.00	0.0176	5.57E-.06	1.80E-07	0.00014	0.7170	0.6420	0.1400	120	Yes	0.2362	0.2171	8.7891
Lindane	8.00	0.0176	5.57E-.06	1.80E-07	0.00014	0.7170	0.6420	0.0900	168	Yes	0.1996	0.1593	25.296

BENZENE 110 PPMW
(1 of 2)

Chemical	Sample Point	Initial soil conc.,	Initial soil conc.,	Flux chamber surface area	Soil Depth	Soil Type	Soil bulk density,	Soil particle density,	Gravimetric soil moisture,	Water-filled soil porosity,	Solubility,	Soil organic carbon,	Saturation conc.,	C_o>C_{sat}	Measured emission flux	Organic carbon part. coeff.,
		C_o	C_o		(L)		ρ_b	ρ_s	w	Θ	S	f_{oc}	C_{sat}		(µg/cm^2	K_{oc}
		(mg/kg)	(g/g)	(cm^2)	(cm)		(Kg/L)	(Kg/L)	(wt. fraction)	(unitless)	(mg/L)	(fraction)	(mg/kg)	(Yes/No)	-day)	(cm^3/g)
Benzene	3	110	1.10E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	1780	0.006	862	No	2760	57
Benzene	4	110	1.10E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	1780	0.006	862	No	9000	57
Benzene	5	110	1.10E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	1780	0.006	862	No	910	57
Benzene	6	110	1.10E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	1780	0.006	862	No	400	57
Benzene	7	110	1.10E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	1780	0.006	862	No	290	57
Benzene	8	110	1.10E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	1780	0.006	862	No	0	57

BENZENE 110 PPMW
(2 of 2)

Chemical	Soil/water part. coeff.,	Diffusivity in air,	Diffusivity in water,	Effective diffusion coefficient,	H	Henry's law constant,	Total soil porosity,	Air-filled soil porosity,	Measured emission flux	Time, t	$t > L^2/14.4\ D_E$	Infinite source model emission flux	Finite source model emmision flux	Infinite source model error
	K_D	D_g^a	D_l^w	D_E		K_H	ϕ	a	(µg/cm^2	Cumulative		(µg/cm^2	(µg/cm^2	
	(cm^3/g)	(cm^2/s)	(cm^2/s)	(cm^2/s)	(atm-m^3/mol)	(unitless)	(unitless)	(unitless)	-day)	(hours)	(Yes/No)	-day)	-day)	(percent)
Benzene	0.34	0.0870	9.80E-06	2.14E-03	0.00543	0.22263	0.4340	0.2840	397	26.40	No	1207	1207	0.0000
Benzene	0.34	0.0870	9.80E-06	2.14E-03	0.00543	0.22263	0.4340	0.2840	1296	76.25	Yes	710	710	0.0002
Benzene	0.34	0.0870	9.80E-06	2.14E-03	0.00543	0.22263	0.4340	0.2840	131	119.73	Yes	567	567	0.0253
Benzene	0.34	0.0870	9.80E-06	2.14E-03	0.00543	0.22263	0.4340	0.2840	58	506.83	Yes	275	209	31.5053
Benzene	0.34	0.0870	9.80E-06	2.14E-03	0.00543	0.22263	0.4340	0.2840	42	698.55	Yes	235	135	73.9743
Benzene	0.34	0.0870	9.80E-06	2.14E-03	0.00543	0.22263	0.4340	0.2840	0	863.17	Yes	211	92	128.3941

TOLUENE 880 PPMW
(1 OF 2)

Chemical	Sample Point	Initial soil conc.	Initial soil conc.	Flux chamber surface area	Soil Depth	Soil Type	Soil bulk density,	Soil particle density,	Gravimetric soil moisture,	Water-filled soil porosity,	Solubility	Soil organic carbon,	Saturation conc.,	$C_o>C_{sat}$	Measured emission flux	Organic carbon part. coeff.,
		C_o	C_o		(L)		ρ_b	ρ_s	w	Θ	S	f_{oc}	C_{sat}		($\mu g/m^2$	K_{oc}
		(mg/kg)	(g/g)	(cm^2)	(cm)		(kg/L)	(kg/L)	(wt. fraction)	(unitless)	(mg/L)	(fraction)	(mg/kg)	(Yes/No)	-min)	(cm^3/g)
Toluene	3	880	8.80E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	558	0.006	522	Yes	14800	131
Toluene	4	880	8.80E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	558	0.006	522	Yes	17300	131
Toluene	5	880	8.80E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	558	0.006	522	Yes	4910	131
Toluene	6	880	8.80E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	558	0.006	522	Yes	1340	131
Toluene	7	880	8.80E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	558	0.006	522	Yes	830	131
Toluene	8	880	8.80E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	558	0.006	522	Yes	340	131
Toluene	9	880	8.80E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	558	0.006	522	Yes	260	131

TOLUENE 880 PPMW
(2 OF 2)

Chemical	Soil/water part. coeff.,	Diffusivity in air,	Diffusivity in water,	Effective diffusion coefficient,	H	Henry's law constant,	Total soil porosity,	Air-filled soil porosity,	Measured emission flux	Time, t	$t > L^2/14.4\ D_E$	Infinite source model emission flux	Finite source model emmision flux	Infinite source model error
	K_D	$D_g{}^a$	$D_i{}^w$	D_E	(atm-	K_H	ϕ	a	(μg/cm$^{2\cdot}$	Cumulative				
	(cm^3/g)	(cm^2/s)	(cm^2/s)	(cm^2/s)	m^3/mol)	(unitless)	(unitless)	(unitless)	day)	(hours)	(Yes/No)	(μg/cm$^{2\cdot}$day)	(μg/cm$^{2\cdot}$day)	(percent)
Toluene	0.79	0.0870	8.60E-06	1.30E-03	0.00637	0.26117	0.4340	0.2840	2131	26.40	No	7524	7524	0.0000
Toluene	0.79	0.0870	8.60E-06	1.30E-03	0.00637	0.26117	0.4340	0.2840	2491	76.25	No	4427	4427	0.0000
Toluene	0.79	0.0870	8.60E-06	1.30E-03	0.00637	0.26117	0.4340	0.2840	707	119.73	No	3533	3533	0.0001
Toluene	0.79	0.0870	8.60E-06	1.30E-03	0 00637	0.26117	0.4340	0.2840	193	506.83	Yes	1717	1613	6.4806
Toluene	0.79	0.0870	8.60E-06	1.30E-03	0.00637	0.26117	0.4340	0.2840	120	698.55	Yes	1463	1231	18.8541
Toluene	0.79	0.0870	8.60E-06	1.30E-03	0.00637	0.26117	0.4340	0.2840	49	863. 17	Yes	1316	978	34.5481
Toluene	0.79	0.0870	8.60E-06	1.30E-03	0.00637	0.26117	0.4340	0.2840	37	1007.17	Yes	1218	800	52.2568

ETHYLBENZENE 310 PPMW
(1 of 2)

Chemical	Sample Point	Initial soil conc.	Initial soil conc.	Flux chamber surface	Soil Depth	Soil Type	Soil bulk density,	Soil particle density,	Gravimetric soil moisture,	Water-filled soil porosity,	Solubility	Soil organic carbon,	Satura-tion conc.,	$C_o>C_{sat}$	Measured emission flux	Organic carbon part. coeff.,
		C_o	C_o	area	(L)		ρ_b	ρ_s	w	Θ	S	f_{oc}	C_{sat}		(μg/cm^2	K_{oc}
		(mg/kg)	(g/g)	(cm^2)	(cm)		(g/cm^3)	(g/cm^3)	(wt. fraction)	(unitless)	(mg/L)	(fraction)	(mg/kg)	(Yes/No)	-min)	(cm^3/g)
Ethylbenzene	3	310	3.1 0E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	173	0.006	257	Yes	2640	221
Ethylbenzene	4	310	3.1 0E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	173	0.006	257	Yes	1700	221
Ethylbenzene	5	310	3.1 0E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	173	0.006	257	Yes	1080	221
Ethylbenzene	6	310	3.1 0E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	173	0.006	257	Yes	250	221
Ethylbenzene	7	310	3.1 0E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	173	0.006	257	Yes	180	221
Ethylbenzene	8	310	3.1 0E-04	1300	91	Loamy Sand	1.5	2.65	0.10	0.1500	173	0.006	257	Yes	0	221

ETHYLBENZENE 310 PPMW
(2 of 2)

Chemical	Soil/ water part. coeff.,	Diffusivity in air,	Diffusivity in water,	Effective diffusion coefficient,	Henry's law constant,	Total soil porosity,	Air-filled soil porosity,	Measured emission flux	Time, t	$t > L^2/14.4\ D_E$	Infinite source model emission flux	Finite source model emmision flux	Infinite source model error
	K_D	D_g^a	D_l^w	D_E	K_H	ϕ	a	(μg/cm^{2-}	Cumulative		(μg/cm^{2-}	(μg/cm^{2-}	
	(cm^3/g)	(cm^2/s)	(cm^2/s)	(cm^2/s)	(unitless)	(unitless)	(unitless)	day)	(hours)	(Yes/No)	day)	day)	(percent)
Ethylbenzene	1.33	0.0750	7.80E-06	8.64E-04	0.32021	0.4340	0.2840	380	26.40	No	2162	2162	0.0000
Ethylbenzene	1.33	0.0750	7.80E-06	8.64E-04	0.32021	0.4340	0.2840	245	76.25	No	1272	1272	0.0000
Ethylbenzene	1.33	0.0750	7.80E-06	8.64E-04	0.32021	0.4340	0.2840	156	119.73	No	1015	1015	0.0000
Ethylbenzene	1.33	0.0750	7.80E-06	8.64E-04	0.32021	0.4340	0.2840	36	506.83	Yes	493	488	1.0596
Ethylbenzene	1.33	0.0750	7.80E-06	8.64E-04	0.32021	0.4340	0.2840	26	698.55	Yes	420	402	4.6357
Ethyibenzene	1.33	0.0750	7.80E-06	8.64E-04	0.32021	0.4340	0.2840	0	863.17	Yes	373	343	10.0850

APPENDIX B

VALIDATION DATA FOR THE JURY REDUCED SOLUTION FINITE SOURCE MODEL

TRIALLATE 10 PPM
(1 OF 2)

Chemical	Sample Point	Initial soil conc.	Initial soil conc.	Emitting	Soil Depth	Soil Type	Soil bulk density,	Soil particle density,	Gravi-metric soil moisture, w	Water-filled soil porosity,	Solubility	Soil organic carbon,	Saturation conc.,	$C_o>C_{sat}$	Measured emission flux	Organic carbon part. coeff.,
		C_o	C_o	area	(L)		ρ_b	ρ_s	(wt.	Θ	S	f_{oc}	C_{sat}		(μg/cm^2	K_{oc}
		(mg/kg)	(g/g)	(cm^2)	(cm)		(Kg/L)	(Kg/L)	fraction)	(unitless)	(mg/L)	(fraction)	(mg/kg)	(Yes/No)	-day)	(cm^3/g)
Triallate	1	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	1.700	3600
Triallate	2	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.975	3600
Triallate	3	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.750	3600
Triallate	4	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.490	3600
Triallate	5	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.330	3600
Triallate	6	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.280	3600
Triallate	7	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.210	3600
Triallate	8	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.180	3600
Triallate	9	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.155	3600
Triallate	10	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.145	3600
Triallate	11	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.135	3600
Triallate	12	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.125	3600
Triallate	13	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.123	3600
Triallate	14	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.115	3600
Triallate	15	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.107	3600
Triallate	16	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.105	3600
Triallate	17	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.103	3600
Triallate	18	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.102	3600
Triallate	19	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.095	3600
Triallate	20	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.094	3600
Triallate	21	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.093	3600
Triallate	22	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.094	3600
Triallate	23	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.085	3600
Triallate	24	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.083	3600
Triallate	25	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.082	3600
Triallate	26	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	1 05	No	0.083	3600
Triallate	27	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.00.72	105	No	0.080	3600
Triallate	28	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.00.72	105	No	0.080	3600
Trlallate	29	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.00.72	105	No	0.072	3600
Triallate	30	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0 071	3600
Triallate	31	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0 070	3600
Triallate	32	10	1.00E-05	30	10	San Joaquin Sandy Loam	1.34	2.65	0.21	0.2787	4.00	0.0072	105	No	0.070	3600

TRIALLATE 10 PPM
(2 OF 2)

Chemical	Soil/ water part. coeff., K_D (cm^3/g)	Diffusivity in air, D_g^a (cm^2/s)	Diffusivity in water, D_l^w (cm^2/s)	Effective diffusion coefficient, D_E (cm^2/s)	Henry's law constant, K_H (unitless)	Total soil porosity, ϕ (unitless)	Air-filled soil porosity, (unitless)	Measured emission flux $(\mu g/cm^2 \cdot day)$	Time, t Cumulative (hours)	Jury finite source model emission flux $(\mu g/cm^2 \cdot day)$
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	1.700	3	1.278
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.975	6	0.904
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.750	12	0.639
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.490	24	0.452
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.330	48	0.320
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.280	72	0.261
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.210	96	0.226
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.180	120	0.202
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.155	144	0.184
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.145	168	0.171
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.135	192	0.160
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.125	216	0.151
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.123	240	0.143
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.115	264	0.136
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.107	288	0.130
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.105	312	0.125
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.103	336	0.121
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.102	360	0.117
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.095	384	0.113
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.094	408	0.110
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.093	432	0.107
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.094	456	0.104
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.085	480	0.101
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.083	504	0.099
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.082	528	0.096
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.083	552	0.094
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.080	576	0.092
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.080	600	0.090
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.072	624	0.085
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.071	648	0.087
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.070	672	0.085
Triallate	25.92	0.0450	5.00E-06	4.14E-08	0.00104	0.4943	0.2156	0.070	696	0.084

APPENDIX D

Revisions to VF and PEF Equations (EQ, 1994b)

ENVIRONMENTAL QUALITY MANAGEMENT, INC.

MEMORANDUM

TO:	Ms. Janine Dinan	**DATE:**	July 11, 1994
SUBJECT:	Revisions to VF and PEF Equations	**FROM:**	Craig Mann
FILE:	5099-3	**cc:**	

Subsequent to the evaluation of the dispersion equations in the RAGS - Part B performed by Environmental Quality Management, Inc. (EQ,1993), questions have arisen as to the accuracy of the modeling protocol used to derive the dispersion coefficient (Q/C) used in the volatilization factor (VF) and the particulate emission factor (PEF) presently employed to calculate the air pathway Soil Screening Levels (SSLs).

EQ, 1993 used the Industrial Source Complex model (ISC2-ST) to derive a normalized concentration (kg/m^3 per g/m^2-s) for a series of square and rectangular area sources of differing size. This modeling protocol employed a source subdivision scheme similar to that recommended in the ISC2-ST Model User's Manual (EPA, 1992) whereby the source was subdivided into smaller sources closest to the center of the area. The center of the area was found to represent the point of maximum annual average concentration for all source shapes analyzed. Consecutive model runs were performed whereby source subdivision was increased between runs. Final source subdivision was reached when the model results converged within a factor of three percent or less.

From these data, a simple linear regression was used to evaluate the nature of the relationship between the normalized concentration and the size of the area. Preliminary plots of the data indicated that the relationship was exponential. Therefore, the relationship was linearized by taking the natural logarithms (ln) of each variable. The resulting linear regression for a square area of 0.5 acres resulted in a normalized concentration (C/Q) of 0.0098 kg/m^3 per g/m^2-s; the inverse of the normalized concentration resulted in a dispersion coefficient (Q/C) of 101.8 g/m^2-s per kg/m^3.

On May 5, 1994 a teleconference was held between representatives of the Toxics Integration Branch of the Office of Emergency and Remedial Response (OERR) and the Source Receptor Analysis Branch of the Office of Air Quality Planning Standards (OAQPS) to discuss the relative merits of the available area source algorithms as applied to nearfield and on-site receptors exposed to ground-level nonbuoyant emissions. The conclusions drawn from this teleconference were that a new algorithm recently developed by OAQPS would yield more accurate results for the exposure scenario in question.

The new algorithm is incorporated into the ISC2 model platform in both short-term mode (AREA-ST) and long-term mode (AREA-LT). Both models employ a double numerical integration over the area source in the upwind and crosswind directions as follows:

$$\chi = \frac{Q_A K}{2\pi u_s} \int_x \frac{VD}{\sigma_y \sigma_z} \left(\int_y \exp\left[-0.5 \left(\frac{Y}{\sigma_y} \right)^2 \right] dy \right) dx \qquad (1)$$

where Q_A = Area source emission rate (g/m^2-s)

K = Units scaling coefficient

V = Vertical term

D = Decay term.

The integral in the lateral (i.e., crosswind or y) direction is solved analytically as:

$$\int_y \exp\left[-0.5\left(\frac{Y}{\sigma_y}\right)^2\right]dy = \operatorname{erfc}\left(\frac{Y}{\sigma_y}\right) \tag{2}$$

where erfc is the complementary error function.

The integral in the longitudinal (i.e., upwind or x) direction is solved by using a weighted average of successive estimates of the integral using a trapezoidal approximation. The model uses three separate criteria to determine convergence of the upwind integral. The result of these numerical methods is an estimate of the full integral that is essentially equivalent to, but much more efficient than, the method of estimating the integral as a series of line sources, such as the method used by the Point, Area, Line (PAL 2.0) model. Wind tunnel tests have also shown that the new algorithm performs well with on-site and near-field receptors.

Because the new algorithm provides better concentration estimates and does not require source subdivision, a revised dispersion analysis was performed for both volatile and particulate matter contaminants using the new algorithm.

The first part of the analysis involved a determination of the relationship between concentration and source size. In addition, this part of the analysis included a determination of the point of maximum annual average concentration for a square area source. This assessment employed the AREA-ST model as acquired from the OAQPS Technology Transfer Network, Support Center for Regulatory Air Models (SCRAM) Bulletin Board.

Meteorological data used for this analysis were 1989 hourly data for the Los Angeles National Weather Service (NWS) surface station, upper air data were from the Oakland NWS station for the same year. Rural dispersion coefficients were employed and all regulatory default options used. Modeling assumed flat terrain with no flagpole receptors; source rotation angle was set equal to zero.

Five source sizes were included in the assessment: 0.5, 5, 30, 200, and 600 acres. A coarse Cartesian receptor grid was employed within and extending beyond the source perimeter; a discrete receptor was also placed at the center of each source (x,y = 0,0). Emissions from each source were set equal to 1.0 g/m^2-s; concentrations were calculated in units of kg/m^3.

Figure 1 shows the relationship between source size (acres) and annual average concentration (kg/m3) for the five source sizes modeled. In each case, the point of maximum concentration was located at the center of the source. As an example, Attachment A is the model run sheets for the 0.5 acre source. As can be seen from Figure 1, the relationship between concentration and source size is exponential. Results also show that the maximum concentration representing the 600 acre source is 2.9 times higher than that of the 0.5 acre source.

Having established that when using the AREA-ST model the point of maximum concentration for a square area source is the center receptor, the second part of the analysis was to determine which of the 29 meteorological sites from EQ, 1993 best represents the average exposure and the high end exposure to volatile and particulate matter emissions. It was determined that the average exposure case should be represented by the 50th percentile site concentration, while the high end exposure is best represented by the 90th percentile site concentration.

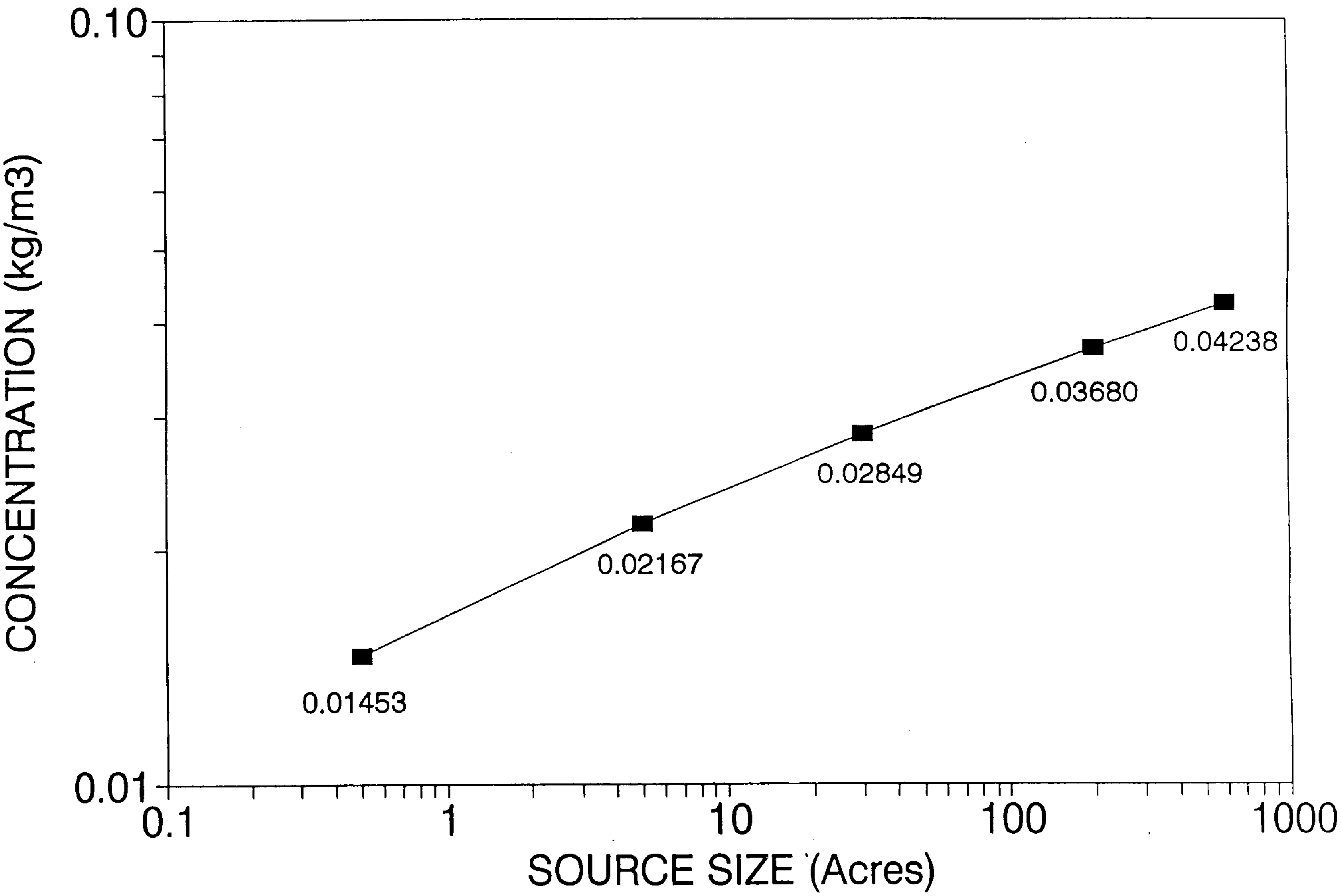


Figure 1
Normalized Annual Average Concentration Versus Source Size

Each of the 29 sites from EQ, 1993 were subsequently modeled at an emission rate of 1.0 g/m^2-s with a single discrete receptor at the center of the square area source. Source sizes modeled were 0.5 acres and 30 acres. Hourly meteorological data for each site were from EQ, 1993. From the set of SS normalized annual average concentrations, the 50th percentile site was determined to be Salt Lake City, Utah; Los Angeles, California (89th percentile site) was determined to be the closest approximation of the 90th percentile site. Table 1 shows the resulting dispersion coefficients for the two source sizes and the percentile ranking of each site.

In order to determine the average and high end sites for particulate matter exposures resulting from wind erosion, a normalized concentration could not be used because meteorological conditions other than simple dispersion (i.e., wind velocity and frequency) influence emissions and therefore actual concentrations. For this reason, actual concentrations were calculated for each site using the existing PEF equation as follows:

$$C = (C/Q)\left[\frac{0.036\,(1-V)\text{ x }(U_m/U_{t-7})^3\text{ x }F(x)}{3600\text{ s/h}}\right] \qquad (3)$$

where C = Annual average PM_{10} concentration, kg/m^3

(C/Q) = Normalized annual average concentration (kg/m^3 per g/m^2 -s)

V = Fraction of continuous vegetative cover

U_m = Mean annual windspeed, m/s

U_{t-7} = Equivalent threshold value of windspeed at 7 m, m/s

F(x) = Windspeed distribution function from Cowherd, 1985.

The value of (C/Q) for each site was the normalized concentration previously estimated for volatile emissions (i.e., the inverse of each dispersion coefficient in Table 1). The value of V was set equal to 0.5. The mean annual windspeed (U_m) for each site was taken from Weather of U.S. Cities, Second Edition, Volume 2 by J. A. Ruffner and F. E. Bair, Gale Research Co., Detroit, Michigan. The value of F(x) was estimated for each site from Figure 4-3 or calculated from Appendix B of Cowherd 1985, as appropriate.

The value of U_{t-7} was calculated as follows:

$$U_{t-7} = \frac{U_t}{0.4}\ln\left(\frac{700}{z_0}\right) \qquad (4)$$

where U_{t-7} = Equivalent threshold value of windspeed at 7 m, m/s

Z_o = Surface roughness height, cm (z_o = 0.5 cm for open terrain)

U_t = Threshold friction velocity, m/s (U_t = 0.625 m/s).

Table 2 gives the results of this analysis and shows the relative PM_{10} concentrations for each site by source size and the percentile rankings. As can be seen from Table 2, the 50th percentile site was Salt Lake City, Utah, while the 89th percentile site was Minneapolis, Minnesota.

TABLE 1.
VOLATILE DISPERSION SITE RANKINGS

City	NWS Surface Station Number	0.5 Acre (Q/C) (g/m^2-s per kg/m^3)	30 Acre (Q/C) (g/m^2-s per kg/m^3)	Site Ranking Percentile (%)
Huntington	13860	52.77	27.08	100
Fresno	93193	62.00	31.85	96
Phoenix	23183	64.06	32.63	93
Los Angeles	**24174**	**68.82**	**35.10**	**89**
Winnemucca	24128	69.25	35.49	86
Boise	24131	69.40	35.69	82
Hartford	14740	71.33	36.64	79
Little Rock	13963	73.37	37.68	75
Portland	14764	74.24	37.86	71
Salem	24232	73.42	37.88	68
Charleston	13880	74.91	38.42	64
Denver	23062	75.59	38.80	61
Atlanta	13874	77.16	39.68	57
Raleigh-Durham	13722	77.46	39.87	54
Salt Lake City	**24127**	**78.06**	**40.14**	**50**
Houston	12960	79.24	40.70	46
Lincoln	14939	81.63	41.56	43
Harrisburg	14751	81.90	42.34	39
Bismarck	24011	83.40	42.72	36
Seattle	24233	82.71	42.81	32
Cleveland	14820	83.19	43.03	29
Albuquerque	23050	84.18	43.31	25
Miami	12839	85.40	43.57	21
San Francisco	23234	89.53	46.06	18
Philadelphia	13739	90.09	46.38	14
Minneapolis	14922	90.74	46.84	11
Las Vegas	23169	95.51	49.48	7
Chicago	94846	97.75	50.45	4
Casper	24089	100.00	51.68	0

TABLE 2. PEF.CALCULATIONS AND SITE RANKINGS

	NWS surface station	Mean annual wind-speed	Mean annual wind-speed	Roughness height, Zo t	Threshold friction velocity at surface	Threshold friction velocity at 7m		F(x),	F(x),	Vegetative cover	PM10 emission flux	0.5 Acre (Q/C) (g/m2-s per	0.5 Acre annual average conc.	30 Acre (Q/C) (g/m2-s per	30 Acre annual average conc.	Site ranking percentile
City	number	(mph)	(m/s)	(cm)	(m/s)	(m/s)	x	x<=2	x>2	(fraction)	(g/m2-s)	kg/m3)	(ug/m3)	kg/ m3)	(ug/ m3)	(%)
Casper	24089	12.9	5.77	0.5	0.625	11.32	1.74	0.57	NA	0.50	3.77E-07	100.00	3.77	51.68	7.29	100
Cleveland	14820	10.8	4.83	0.5	0.625	11.32	2.08	NA	2.32E-01	0.50	9.01E-08	83.19	1.08	43.03	2.09	96
Lincoln	14939	10.4	4.65	0.5.	0.625	11.32	2.16	NA	1.82E-01	0.50	6.30E-08	81.63	077	41.56	1.52	93
Minneapolis	**14922**	**10.5**	**4.69**	**0.5**	**0.625**	**11.32**	**2.14**	**NA**	**1.94E-01**	**0.50**	**6.92E-08**	**90.74**	**0.76**	**46.84**	**1.48**	**89**
Bismarck	24011	10.3	4.60	0.5	0.625	11.3Z	2.18	NA	1.70E-01	0.50	5.73E-08	83.40	0.69	42.72	1.34	86
Chicago	94846	10.4	4.65	0.5	0.625	11.32	2.16	NA	1.82E-01	0.50	6.30E-08	97.75	0.64	50.45	1.25	82
Philadelphia	13739	9.6	4.29	0.5	0.625	11.32	2.34	NA	9.93E-02	0.50	2.71E-08	90.09	0.30	46.38	0.58	79
Miami	12835	9.2	4.11	0.5	0.625	11.32	2.44	NA	6.82E-02	0.50	1.64E-08	85.40	0.19	43.57	0.38	75
Altanta	13874	9.1	4.07	0.5	0.625	11.32	2.47	NA	6.16E-02	0.50	1.43E-08	77.16	0.19	39.68	0.36	71
Seattle	24233	9.1	4.07	0.5	0.625	11.32	2.47	NA	6.16E-02	0.50	1.43E-08	82.71	0.17	42.81	0.33	68
Boise	24131	8.9	3.98	0.5	0.625	11.32	2.52	NA	4.95E-02	0.50	1.07E-08	69.40	0.15	35.69	0.30	64
Las Vegas	23165	9.1	4.07	0.5	0.625	11.32	2.47	NA	6.16E-02	0.50	1.43E-08	95.51	0.15	49.48	0.29	61
Albuquerque	23050	9.0	4.02	0.5	0.625	11.32	2.49	NA	5.53E-02	0.50	1.24E-08	84.18	0.15	43.31	0.29	57
Denver	23062	8.8	3.93	0.5	0.625	11.32	2.55	NA	4.41E-02	0.50	9.25E-09	75.59	0.12	38.80	0.24	54
Salt Lake City	**24127**	**8.8**	**3.93**	**0.5**	**0.625**	**11.32**	**2.55**	**NA**	**4.41E-02**	**0.50**	**9.25E-09**	**78.06**	**0.12**	**40.14**	**0.23**	**50**
Portland	14762	8.7	3.89	0.5	0.625	11.32	2.58	NA	3.91E-02	0.50	7.93E-09	74.24	0.11	37.86	0.21	46
Charleston	13880	8.7	3.89	0.5	0.625	11.32	2.58	NA	3.91E-02	0.50	7.93E-09	74.91	0.11	38.42	0.21	43
Hartford	14764	8.6	3.84	0.5	0.625	11.32	2.61	NA	3.45E-02	0.50	6.76E-09	71.33	0.095	36.64	0.18	39
San Francisco	23234	8.7	3.89	0.5	0.625	11.32	2.58	NA	3.91E-02	0.50	7.93E-09	89.53	0.089	46.06	0.17	36
Little Rock	13963	8.0	3.58	0.5	0.625	11.32	2.80	NA	1.45E-02	0.50	2.29E-09	73.37	0.031	37.68	0.061	32
Winnemucca	24128	7.9	3.53	0.5	0.625	11.32	2.84	NA	1.23E-02	0.50	1.86E-09	69.25	0.027	35.49	0.052	29
Houston	12960	7.8	3.49	0.5	0.625	11.32	2.88	NA	1.03E-02	0.50	1.51E-09	79.24	0.019	40.70	0.037	25
Raleigh-Durham	13722	7.7	3.44	0.5	0.625	11.32	2.91	NA	8.60E-03	0.50	1.21E-09	77.461	0.016	39.87	0.030	21
Harrisburg	14751	7.7	3.44	0.5	0.625	11.32	2.91	NA	8.60E-03	0.50	1.21E-09	81.90	0.015	42.34	0.029	18
LosAngeles	24174	7.4	3.31	0.5	0.625	11.32	3.03	NA	4.74E-03	0.50	5.92E-10	68.82	8.60E-03	35.10	0.017	14
Salem	2423 2	7.0	3.13	0.5	0.625	11.32	3.21	NA	1.87E-03	0.50	1.98E-10	73.42	2.69E-03	37.88	5.22E-03	11
Huntington	13860	6.5	2.91	0.5	0.625	11.32	3.45	NA	4.45E-04	0.50	3.76E-11	52.77	7.13E-04	27.08	1.39E-03	7
Fresno	93193	6.4	2.86	0.5	0.625	11.32	3.51	NA	3.19E-04	0.50	2.58E-11	62.00	4.16E-04	31.85	8.09E-04	4
Phoenix	23183	6.3	2.82	0.5	0.625	11.32	3.56	NA	2.25E-04	0.50	1.73E-11	64.06	2.71E-04	32.63	5.31E-04	0

F(x) <= 2 from Cowherd (1985), Figure 4-3.
F(x) > 2 from Cowherd (1985), Appendix B.
NA = Not Appilcable.

Table 3 summarizes the results of the dispersion coefficient analysis for both the VF and PEF equations. In addition, Table 3 also gives the default values of the PEF variables for both average and high end exposures.

TABLE 3.
VF AND PEF VALUES OF (Q/C) FOR AVERAGE AND HIGH END EXPOSURES

Site size	Average annual conc., PM10 (ug/m^3)	High End annual conc., PM10 (ug/m^3)	PEF Average (Q/C), (g/m^2-s per kg/m^3)	PEF High End (Q/C), (g/m^2-s per kg/m^3)	VF Average (Q/C), (g/m^2-s per kg/m^3)	VF High End (Q/C), (g/m^2-s per kg/m^3)
0.5 Acres	0.12	0.76	78.06	90.74	78.06	68.82
30 Acres	0.23	1.48	40.14	46.84	40.14	35.10

Average Site for PM10= Salt Lake City
Average Site for Volatiles = Salt Lake City
High End Site for PM10 = Minneapolis
High End Site for Volatiles = Los Angeles

Average Site for PM10: Mean annual windspeed (U_m) = 3.93 m/s; F(x) = 0.044, at x = 2.55.
High End Site for PM10: U_m = 4.69 m/s; F(x) = 0.194, at x = 2.14.
Where:
Vegetative cover (V) = 0.5.
Surface roughness height (Z_o) = 0.5 cm.
Threshold friction velocity (U_t) = 0.625 m/s at surface.
Threshold windspeed at 7 meters (U_t-7) = U_t/0.4 x ln(700/Z_o) = 11.32 m/s.

ATTACHMENT A

AREA-ST MODEL RUN SHEETS FOR A 0.5 ACRE SQUARE AREA SOURCE

```
CO      STARTING
CO      TITLEONE       AREA    SOURCES--- 1/2 acre    run
CO      MODELOPT       DFAULT  CONC     RURAL
CO      AVERTIME       PERIOD
CO      POLLUTID       PM10
CO      RUNORNOT       RUN
CO      ERRORFIL       AREA1.ERR
CO      FINISHED


SO STARTING
                SRCID       SRCTYP      XS          YS          ZS
SO LOCATION     A1/2        AREA        -22.5       -22.5       .0000
                SRCID       QS          HS          XINIT       YINIT
SO SRCPARAH     A1/2        1.0         0.0         45.         45.

SO      EHISUNIT       .100000E-02    (GRAMS/(SEC-M**2))    KILOGRAMS/CUBIC-METER

SO      SRCGROUP       AREA1   A1/2

SO      FINISHED

RE      STARTING
RE      DISCCART       0.             o.
RE      DISCCART       25.            0.
RE      DISCCART       -25.           o.
RE      DISCCART       25.            25.
RE      DISCCART       25.            -25.
RE      DISCCART       -25.           -25.
RE      DISCCART       -25.           25.
RE      DISCCART       50.            0.
RE      DISCCART       -50.           0.
RE      DISCCART       50.            50.
RE      DISCCART       50.            -50.
RE      DISCCART       -50.           -50.
RE      DISCCART       -50.           50.
RE      DSSCCART       75.            0.
RE      DISCCART       -75.           0.
RE      DISCCART       75.            75.
RE      DISCCART       75.            -75.
RE      DISCCART       -75.           -75.
RE      DISCCART       -75.           75.
RE      DISCCART       100.           0.
RE      DISCCART       -100.          0.
RE      DISCCART       100.           100.
RE      DISCCART       100.           -100.
RE      DISCCART       -100.          -100.
RE      DISCCART       -100.          100.

RE      FINISHED

ME      STARTING
ME      INPUTFIL       C:\CRAIG\23174-89.ASC
ME      ANEHHGHT       10.0 METERS
ME      SURFDATA       23174  1989    LOS ANGELES
ME      UAIRDATA       23230  1989    OAKLAND
```

```
ME      WINDCATS       1.54    3.09    5.14    8.23    10.80
ME      FINISHED

OU      STARTING
OU      RECTABLE       ALLAVE  FIRST
OU      FINISHED

***************************************************
*** SETUP Finishes Successfully ***
***************************************************
```

```
*** AREAST - VERSION TESTA ***   *** AREA SOURCES---1/2 acre run***
TEST OF ST AREA SOURCE ALGORITHM ***                            ***

*** MODELING OPTIONS USED: CONC RURAL FLAT DFAULT

                           *** MODEL SETUP OPTIONS SUMMARY     ***

**Model Is Setup For Calculation of Average CONCentration Values.

**Model Uses RURAL Dispersion.

**Model Uses Regulatory DEFAULT Options:
       1. Final Plume Rise.
       2. Stack-tip Downwash.
       3. Buoyancy-induced Dispersion.
       4. Use Calms Processing Routine.
       5. Not Use Missing Data Processing Routine.
       6. Default Wind Profile Exponents.
       7. Default Vertical Potential Temperature Gradients.
       8. “Upper Bound” Values for Supersquat Buildings.
       9. No Exponential Decay for RURAL Mode

**Model Assumes Receptors on FLAT Terrain.

**Model Assumes No FLAGPOLE Receptor Heights.

**Model Calculates PERIOD Averages Only

**This Run Includes: 1 Source(s); 1 Source Group(s); and 25 Receptore(s)

**The Model Assumes A Pollutant Type of: PM10

**Model Set To Continue RUNning After the Setup Testing.ff

**Output Options Selected:
Model Outputs Tables of PERIOD Averages by Receptor
Model Outputs Tables of Highest Short Term Values by Receptor (RECTABLE Keyword)

**NOTE: The Following Flags May Appear Following CONC Values:
       c for Calm Hours
       m for Hissing Hours
       b for Both Calm and Missing Hours

**Misc. Inputs:
       Anem. Hgt. (m) = 10.00 ; Decay Coef. =.0000 ; Rot. Angle = .0
       Emission Units = (GRAMS/(SEC-M**2)); Emission Rate Unit Factor = .lOOOOE-02
       Output Units = KILOGRAMS/CUBIC-METER

**input Runstream File: area1.dat,                  **Output Print File: area1.out
**Detailed Error/Message File: AREA1.ERR
```

```
*** AREAST - VERSION TESTA ***   *** AREA SOURCES--- 1/2 acre run                        ***
TEST OF ST AREA SOURCE ALGORITHM ***                                                     ***

*** MODELING OPTIONS USED: CONC RURAL FLAT          DFAULT


                                   *** AREA SOURCE DATA ***

SOURCE   NUMBER   EMISSION RATE   COORD      (SW CORNER)   BASE       RELEASE    X-DIM OF   Y-DIM OF   ORIENT.   EMISSION
ID       PART.    (USER UNITS     X          Y             ELEV.      HEIGHT     AREA       AREA       OF AREA   RATE SCALAR
         CATS.    /METERS**2)     (METERS)   (METERS)      (METERS)   (METERS)   (METERS)   (METERS)   (DEG.)    VARY BY
-----------------------------------------------------------------------------------------------------------------------------
A1/2     0        .10000E+01      -22.5      -22.5         .0         .00        45.00      45.00      .00

*** AREAST - VERSION TESTA ***    *** AREA SOURCES--- 1/2 acre run                       ***
TEST OF ST AREA SOURCE ALGORITHM  ***                                                    ***

*** MODELING OPTIONS USED: CONC RURAL FLAT DFAULT


                         *** SOURCE IDs DEFINING SOURCE GROUPS ***

GROUP ID                                    SOURCE IDs


AREA1 A1/2
```

```
*** AREAST - VERSION TESTA *** *** AREA SOURCES--- 1/2 acre run
TEST OF ST AREA SOURCE ALGORITHM ***        ***

*** MODELING OPTIONS USED: CONC RURAL FLAT DFAULT



                       *** DISCRETE CARTESIAN RECEPTORS ***
                     (X-COORD, Y-C00RD, ZELEV, ZFLAG) (METERS)

         (       .0,       .0,   .0,     .0);   (     25.0,       .0,   .0,     .0);
         (   -25.0,       .0,   .0,     .0);   (     25.0,     25.0,   .0,     .0);
         (    25.0    -25.0,   .0,     .0);   (    -25.0,    -25.0,   .0,     .0);
         (   -25.0     25.0,   .0,     .0);   (     50.0,       .0,   .0,     .0);
         (   -50.0,       .0,   .0,     .0);   (     50.0,     50.0,   .0,     .0);
         (    50.0    -50.0,   .0,     .0);   (    -50.0,    -50.0,   .0,     .0);
         (   -50.0     50.0,   .0,     .0);   (     75.0,       .0,   .0,     .0);
         (   -75.0,       .0,   .0,     .0);   (     75.0,     75.0,   .0,     .0);
         (    75.0,    -75.0,   .0,     .0);   (    -75.0,    -75.0,   .0,     .0);
         (   -75.0,     75.0,   .0,     .0);   (    100.0,       .0,   .0,     .0);
         (  -100.0,       .0,   .0,     .0);   (    100.0,    100.0,   .0,     .0);
         (   100.0,    100.0,   .0,     .0);   (   -100.0,   -100.0,   .0,     .0);
         (  -100.0,    100.0,   .0,     .0);
```

```
*** AREAST - VERSION TESTA *** *** AREA SOURCES--- 1/2 acre run
TEST OF ST AREA SOURCE ALGORITHM ***                ***

*** MODELING OPTIONS USED CONC RURAL FLAT DFAULT


                      *** METEOROLOGICAL DAYS SELECTED FOR PROCESSING ***
                                        (1=YES; 0=NO)

1111111111      1111111111      1111111111      1111111111      1111111111
1111111111      1111111111      1111111111      1111111111      1111111111
1111111111      1111111111      1111111111      1111111111      1111111111
1111111111      1111111111      1111111111      1111111111      1111111111
1111111111      1111111111      1111111111      1111111111      1111111111
1111111111      1111111111      1111111111      1111111111      1111111111
1111111111      111111

NOTE: METEOROLOGICAL DATA ACTUALLY PROCESSED WlLL ALSO DEPEND ON WHAT IS INCLUDED IN THE DATA FILE

                *** UPPER BOUND OF FIRST THROUGH FIFTH WIND SPEED CATEGORIES ***
                                        (HETERS/SEC)

                              1.54, 3.09, 5.14, 8.23, 10.80,

                              *** WIND PROFILE EXPONENTS ***

STABILITY                                 WlND SPEED CATEGORY
CATEGORY          1              2              3              4              5              6
    A       .70000E-01     .70000E-01     .70000E-01     .70000E-01     .70000E-01     .70000E-01
    B       .70000E-01     .70000E-01     .70000E-01     .70000E-01     .70000E-01     .70000E-01
    C       .10000E+00     .10000E+00     .10000E+00     .10000E+00     .10000E+00     .10000E+00
    D       .15000E+00     .15000E+00     .15000E+00     .15000E+00     .15000E+00     .15000E+00
    E       .35000E+00     .35000E+00     .35000E+00     .35000E+00     .35000E+00     .35000E+00
    F       .55000E+00     .55000E+00     .55000E+00     .55000E+00     .55000E+00     .55000E+00


                     *** VERTICAL POTENTIAL TEMPERATURE GRADIENTS ***
                                 (DEGREES KELVIN PER METER)

STABILITY                                 WIND SPEED CATEGORY
CATEGORY          1              2              3              4              5              6
    A       .00000E+00     .O0000E+00     .00000E+00     .00000E+00     .00000E+00     .O0000E+00
    B       .00000E+00     .00000E+00     .00000t+00     .00000E+00     .00000E+OO     .00000E+OO
    C       .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00
    D       .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00     .OO000E+00
    E       .20000E-01     .20000E-01     .20000E-01     .20000E-01     .20000E-01     .20000E-01
    F       .35000E-01     .35000E-01     .35000E-01     .35000E-01     .35000E-01     .35000E-01
```

```
*** AREAST - VERSION TESTA ***    *** AREA SOURCES--- 1/2 acre run                                  ***
TEST OF ST AREA SOURCE ALGORITHM  ***                                                               ***

*** MODELING OPTIONS USED: CONC RURAL FLAT DFAULT


                       *** THE FIRST 24 HOURS OF METEOROLOGICAL DATA ***

FILE: C:\CRAIG\23174-89.ASC                       FORMAT: (4I2,2F9.4,F6.1,I2,2F7.1)
SURFACE STATION NO : 23174                        UPPER AIR STATION NO.: 23230
NAME: LOS                                         NAME: OAKLAND
YEAR: 1989                                        YEAR: 1989

YEAR    MONTH   DAY     HOUR    FLOW     SPEED    TEMP     STAB     MIXING    HEIGHT (M)
                                VECTOR   (M/S)    (K)      CLASS    RURAL     URBAN
89      1       1       1       251.0    3.09     282.6    4        533.0     533.0
89      1       1       2       228.0    3.09     282.0    4        568.6     568.6
89      1       1       3       194.0    2.57     282.0    4        604.1     604.1
89      1       1       4       143.0    4.63     282.0    4        639.6     639.6
89      1       1       5       173.0    2.06     282.0    5        675.2     151.0
89      1       1       6       272.0    3.09     280.4    6        710.7     151.0
89      1       1       7       265.0    2.06     280.4    6        746.3     151.0
89      1       1       8       233.0    2.06     282.0    5        134.9     265.4
89      1       1       9       257.0    2.06     283.7    4        278.2     387.0
89      1       1       10      261.0    .00      285.9    3        421.6     508.6
89      1       1       11      44.0     2.06     288.2    3        564.9     630.2
89      1       1       12      56.0     3.60     289.3    3        708.3     751.8
89      1       1       13      83.0     4.12     289.3    3        851.6     873.4
89      1       1       14      59.0     4.12     290.4    3        995.0     995.0
89      1       1       15      82.0     4.12     287.6    3        995.0     995.0
89      1       1       16      74.0     3.60     287.6    4        995.0     995.0
89      1       1       17      81.0     3.60     285.9    5        992.3     979.1
89      1       1       18      87.0     3.09     284.3    6        975.8     880.6
89      1       1       19      154.0    4.12     286.5    5        959.2     782.2
89      1       1       20      167.0    2.06     285.4    6        942.7     683.8
89      1       1       21      280.0    2.57     285.4    6        926.2     585.3
89      1       1       22      252.0    2.06     284.3    6        909.6     486.9
89      1       1       23      220.0    3.09     283.2    6        893.1     388.4
89      1       1       24      260.0    1.54     283.7    7        876.5     290.0

*** NOTES: STABILITY CLASS 1=A, 2=B, 3=C, 4=D, 5=E AND 6=F.
           FLOW VECTOR IS DIRECTION TOWARD WHICH WIND IS BLOWING.
```

```
*** AREAST - VERSION TESTA ***   *** AREA SOURCES--- 1/2 acre run                  ***
TEST OF ST AREA SOURCE ALGORITHM ***                                               ***

*** MODELING OPTIONS USED: CONC RURAL FLAT      DFAULT

 *** THE PERIOD ( 8760 HRS) AVERAGE CONCENTRATION VALUES FOR SOURCE GROUP: AREA1 ***
 INCLUDING SOURCE(S): A1/2,

                          *** DISCRETE CARTESIAN RECEPTOR POINTS ***


 ** CONC OF PM10                 IN KILOGRAMS/CUBIC-METER                            **


X-COORD (M)      Y-COORD (M)      CONE             X-COORD (M))     Y-COORD (M       CONC
.00              .00              .01453           25.00            .00              .00679
-25.00           .00              .00594           25.00            25.00            .00414
25.00            -25.00           .00104           -25.00           -25.00           .00220
-25.00           25.00            .00223           50.00            .00              .00175
-50.00           .00              .00158           50.00            50.00            .00060
50.00            -50.00           .00018           -50.00           -50.00           .00034
-50.00           50.00            .00037           75.00            .00              .00076
-75.00           .00              .00078           75.00            75 .00           .00024
75.00            -75.00           .00008           -75.00           -75.00           .00015
-75.00           75.00            .00016           100.00           .00              .00041
-100.00          .00              .00047           100.00           100.00           .00013
100.00           -100.00          .00005           -100.00          -100.00          .00009
-100.00          100.00           .00009
```

```
*** AREAST - VERSION TESTA ***   *** AREA SOURCES--- 1/2 acre run
TEST OF ST AREA SOURCE ALGORITHM ***

*** MODELING OPTIONS USED: CONC RURAL FLAT           DFAULT

                  *** THE SUMMARY OF MAXIMUM PERIOD ( 8760 HRS) RESULTS ***

                    ** CONC OF PM10IN    KILOGRAMS/CUBIC-METER         **

                                                                                         NETWORK
GROUP ID             AVERAGE CONC           RECEPTOR (XR, YR, ZELEV, ZFLAG) OF TYPE GRID-ID

AREA1   1ST HIGHEST VALUE IS   .01453 AT (       .00,         .00,   .00,       .00)      DC
        2ND HIGHEST VALUE IS   .00679 AT (     25.00,         .00,   .00,       .00)      DC
        3RD HIGHEST VALUE IS   .00594 AT (    -25.00,         .00,   .00,       .00)      DC
        4TH HIGHEST VALUE IS   .00414 AT (     25.00,       25.00,   .00,       .00)      DC
        5TH HIGHEST VALUE IS   .00223 AT (    -25.00,       25.00,   .00,       .00)      DC
        6TH HIGHEST VALUE IS   .00220 AT (    -25.00,      -25.00,   .00,       .00)      DC

*** RECEPTOR TYPES:
GC = GRIDCART
GP = GRIDPOLR
DC = DISCCART
DP = DISCPOLR
BD = BOUNDARY
```

```
*** AREAST - VERSION TESTA ***   *** AREA SOURCES--- 1/2 acre run                        ***
TEST OF ST AREA SOURCE ALGORITHM ***                                                      ***

*** MODELING OPTIONS USED: CONC RURAL FLAT        DFAULT

*** Message Summary For ISC2 Model Execution ***

 -------- Summary of Total Messages --------

A Total of       0 Fatal Error Message(s)
A Total of       0 Warning Message(s)
A Totat of     653 Informational Message(s)

A Total of     653 Calm Hours Identified


                            ******** FATAL ERROR MESSAGES ********
                                         *** NONE ***

                              ******** WARNING MESSAGES ********
                                         *** NONE ***

                         ********************************************
                          *** ISCST2 Finishes Successfully ***
                         ********************************************
```

APPENDIX E

Determination of Ground Water Dilution Attenuation Factors

DETERMINATION OF GROUNDWATER DILUTION ATTENUATION FACTORS FOR FIXED WASTE SITE AREAS USING EPACMTP

BACKGROUND DOCUMENT

EPA OFFICE OF SOLID WASTE

May 11, 1994

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

PREFACE

The work documented in this report was conducted by HydroGeoLogic, Inc. for the EPA Office of Solid Waste. The work was performed partially under Contract No. 68-W0-0029 and partially under Contract No. 68-W3-0008, subcontracted through ICF Inc. This documentation was prepared under Contract No. 68-W4-0017. Technical direction on behalf of the Office of Solid Waste was provided by Dr. Z.A. Saleem.

ABSTRACT

The EPA Composite Model for Leachate Migration with Transformation Products (EPACMTP) was applied to generate Dilution Attenuation Factors (DAF) for the groundwater pathway in support of the development of Soil Screening Level Guidance. The model was applied on a nationwide basis, using Monte Carlo simulation, to determine DAFs as a function of the area of the contaminated site at various probability levels. The analysis was conducted in two stages: First, the number of Monte Carlo iterations required to achieve converged results was determined. Convergence was defined as a change of less than 5 % in the 85th percentile DAF value. A number of 15,000 Monte Carlo iterations was determined to yield convergence; subsequent analyses were performed using this number of iterations. Second, Monte Carlo analyses were performed to determine DAF values as a function of the contaminated area. The effects of different placements of the receptor well were evaluated.

1.0 INTRODUCTION

The Agency is developing estimates for threshold values of chemical concentrations in soils at contaminated sites that represent a level of concentration above which there is sufficient concern to warrant further site-specific study. These concentration levels are called Soil Screening Levels (SSLs). The primary purpose of the SSLs is to accelerate decision making concerning contaminated soils. Generally, if contaminant concentrations in soil fall below the screening level and the site meets specific residential use conditions, no further study or action is warranted for that area under CERCLA (EPA, 1993b).

The Soil Screening Levels have been developed using residential land use human exposure assumptions and considering multiple pathways of exposure to the contaminants, including migration of contaminants through soil to an underlying potable aquifer. Contaminant migration through the unsaturated zone to the water table generally reduces the soil leachate concentration by attenuation processes such as adsorption and degradation. Groundwater transport in the saturated zone further reduces concentrations through attenuation and dilution. The contaminant concentration arriving at a receptor point in the saturated zone, e.g., a domestic drinking water well, is therefore generally lower than the original contaminant concentration in the soil leachate.

The reduction in concentration can be expressed succinctly in a Dilution-Attenuation Factor (DAF) defined as the ratio of original soil leachate concentration to the receptor point concentration. The lowest possible value of DAF is therefore one; a value of DAF=1 means that there is no dilution or attenuation at all; the concentration at the receptor point is the same as that in the soil leachate. High values of DAF on the other hand correspond to a high degree of dilution and attenuation.

For any specific site, the DAF depends on the interaction of a multitude of site-specific factors and physical and bio-chemical processes. The DAF also depends on the nature of the contaminant itself; i.e., whether or not the chemical degrades or sorbs. As a result, it is impossible to predict DAF values without the aid of a suitable computer fate and transport simulation model that simulates the migration of a contaminant through the subsurface, and accounts for the relevant mechanisms and processes that affect the receptor concentration.

The Agency has developed the EPA Composite Model for Leachate Migration with Transformation Products (EPACMTP; EPA, l993a, 1994) to assess the groundwater quality impacts due to migration of wastes from surface waste sites. This model simulates the fate and transport of contaminants after their release from the land disposal unit into the soil, downwards to the water table and subsequently through the saturated zone. The fate and transport model has been coupled to a Monte Carlo driver to permit determination of DAFs on a generic, nationwide basis. The EPACMTP model has been applied to determine DAFs for the subsurface pathway for fixed waste site areas, as part of the development of Soil Screening Levels. This report describes the application of EPACMTP for this purpose.

2.0 GROUNDWATER MODEL

2.1 Description of EPACMTP Model

The EPA Composite Model for Leachate Migration with Transformation Products (EPACMTP, EPA, 1993a, 1994) is a computer model for simulating the subsurface fate and transport of contaminants that are released at or near the soil surface. A schematic view of the conceptual subsurface system as simulated by EPACMTP, is shown in Figure 1. The contaminants are initially released over a rectangular source area representing the waste site. The modeled subsurface system consists of an unsaturated zone underneath the source area, and an underlying water table aquifer. Contaminants move vertically downward through the unsaturated zone to the water table. The contaminant is assumed to be dissolved in the aqueous phase; it migrates through the soil under the influence of downward infiltration. The rate of infiltration may reflect the combined effect of precipitation and releases from the source area. Once the contaminant enters the saturated zone, a three-dimensional plume develops under the combined influence of advection with the ambient groundwater flow and dispersive mixing.

The EPACMTP accounts for the following processes affecting contaminant fate and transport: advection, dispersion, equilibrium sorption, first-order decay reactions, and recharge dilution in the saturated zone. For contaminants that transform into one or more daughter products, the model can account for the fate and transport of those transformation products also.

The EPACMTP model consists of three main modules:

- An unsaturated zone flow and transport module
- A saturated zone flow and transport module
- A Monte Carlo driver module, which generates model input parameter values from specified probability distributions

The assumptions of the unsaturated zone and saturated zone flow and transport modules are described in Section 2.2. The Monte Carlo modeling procedure is described in Section 2.3.

2.2 Fate and Transport Simulation Modules

2.2.1 Unsaturated zone flow and transport module

Details on the mathematical formulation and solution techniques of the unsaturated zone flow and transport module are provided in the EPACMTP background document (EPA, 1993a). For completeness, the major features and assumptions are summarized below:

- The source area is a rectangular area.
- Contaminants are distributed uniformly over the source area.
- The soil is a uniform, isotropic porous medium.
- Flow and transport in the unsaturated zone are one-dimensional, downward.
- Flow is steady state, and driven by a prescribed rate of infiltration.
- Flow is isothermal and governed by Darcy's Law.

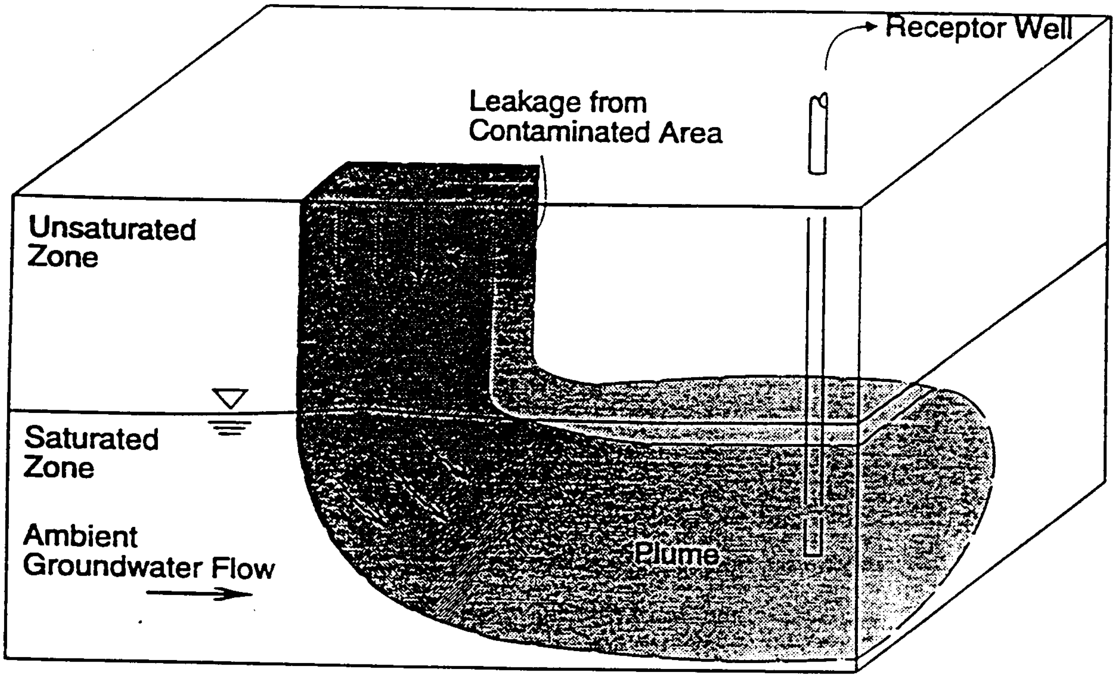


Figure 1
Conceptual View Of The Unsaturated Zone-Saturated Zone System Simulated By EPACMTP

- The leachate concentration entering the soil is either constant (with a finite or infinite duration), or decreasing with time following a first-order decay process.
- The chemical is dilute and present in solution or soil solid phase only.
- Sorption of chemicals onto the soil solid phase is described by a linear or nonlinear (Freundlich) equilibrium isotherm.
- Chemical and biological transformation process can be represented by an effective, first-order decay coefficient.

2.2.2 Saturated zone flow and transport module

The unsaturated zone module computes the contaminant concentration arriving at the water table, as a function of time. Multiplying this concentration by the rate of infiltration through the unsaturated zone yields the contaminant mass flux entering the saturated zone. This mass flux is specified as the source boundary condition for the saturated zone flow and transport module.

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

In addition to modeling fully three-dimensional groundwater flow and contaminant fate and transport, EPACMTP offers the option to perform quasi-3D modeling. When this option is selected, the model ignores either the flow component in the horizontal transverse (-y) direction, or the vertical (-z) direction. The appropriate 2D approximation is selected automatically in the code, based on the relative significance of plume movement in the horizontal transverse versus vertical directions. Details of this procedure are provided in the saturated zone background document (EPA, 1993a). The switching criterion that is implemented in the code will select the 2D areal solution for situations with a relatively thin saturated zone in which the contaminant plume would occupy the entire saturated thickness; conversely, the solution in which advection in the horizontal transverse direction is ignored is used in situations with a large saturated thickness, in which the effect of vertical plume movement is more important.

The saturated zone transport module describes the advective-dispersive transport of dissolved contaminants in a three-dimensional, constant thickness aquifer. The initial boundary is zero, and the lower aquifer boundary is taken to be impermeable. No-flux conditions are set for the upstream aquifer boundary. Contaminants enter the saturated zone through a patch source of either constant concentration or constant mass flux on the upper aquifer boundary, representing the area directly underneath the waste site at the soil surface. The source may be of a finite or infinite duration. Recharge of contaminant-free infiltration water occurs along the upper aquifer boundary outside the patch source. Transport mechanisms considered are advection, longitudinal, vertical and transverse hydrodynamic dispersion, linear or nonlinear equilibrium adsorption, first-order decay and daughter product formation. As in the unsaturated zone, the saturated zone transport module can simulate multi-species transport involving chained decay reactions. The saturated zone transport module of EPACMTP can perform either a fully three-dimensional transport simulation, or provide a quasi-3D approximation. The latter ignores advection in either the horizontal transverse (-y) direction, on the vertical (-z) direction, consistent with the quasi-3D flow solution. In the course of a Monte Carlo simulation, the appropriate 2D approximations are selected automatically for each individual Monte Carlo iteration, thus yielding an overall quasi-3D simulation.

The saturated zone and transport module is based on the following assumptions:

- The aquifer is uniform and initially contaminant-free.
- The flow field is at steady state; seasonal fluctuations in groundwater flow are neglected.
- The saturated thickness of the aquifer remains constant; mounding is represented by the head distribution along the top boundary of the modeled saturated zone system.
- Flow is isothermal and governed by Darcy's Law.
- The chemical is dilute and present in the solution or aquifer solid phase only.
- Adsorption onto the solid phase is described by a linear or nonlinear equilibrium isotherm.
- Chemical and/or biochemical transformation of the contaminant can be described as a first-order process.

2.2.3 Model capabilities and limitations

EPACMTP is based on a number of simplifying assumptions which make the code easier to use and ensure its computational efficiency. These assumptions, however, may cause application of the model to be inappropriate in certain situations.

The main assumptions embedded in the fate and transport model are summarized in the previous sections and are discussed in more detail here. The user should verify that the assumptions are reasonable for a given application.

Uniform Porous Soil and Aquifer Medium. EPACMTP assumes that the soil and aquifer behave as uniform porous media and that flow and transport are described by Darcy's law and the advection-dispersion equation, respectively. The model does not account for the presence of cracks, macro-pores, and fractures. Where these features are present, EPACMTP may underpredict the rate of contaminant movement.

Single Phase Flow and Transport. The model assumes that the water phase is the only mobile phase and disregards interphase transfer processes other than reversible adsorption onto the solid phase. For example, the model does not account for volatilization in the unsaturated zone, which will tend to give conservative predictions for volatile chemicals. The model also does not account for the presence of a second liquid phase (e.g., oil). When a mobile oil phase is present, the movement of hydrophobic chemicals may be underpredicted by the model, since significant migration may occur in the oil phase rather than in the water phase.

Equilibrium Adsorption. The model assumes that adsorption of contaminants onto the soil or aquifer solid phase occurs instantaneously, or at least rapidly relative to the rate of contaminant movement. In addition, the adsorption process is taken to be entirely reversible.

Geochemistry. The EPACMTP model does not account for complex geochemical processes, such as ion exchange, precipitation and complexation, which may affect the migration of chemicals in the subsurface environment. EPACMTP can only approximate such processes as an effective equilibrium retardation process. The effect of geochemical interactions may be especially important in the fate and transport analyses of metals. Enhancement of the model for handling a wide variety of geochemical conditions is currently underway.

First-Order Decay. It is assumed that the rate of contaminant loss due to decay reactions is proportional to the dissolved contaminant concentration. The model is based on one overall decay constant and does not explicitly account for multiple degradation processes, such as oxidation, hydrolysis, and biodegradation. When multiple decay processes do occur, the user must determine the overall, effective decay rate. In order to increase flexibility of the model, the user may instruct the model to determine the overall decay coefficient from chemical specific hydrolysis constants plus soil and aquifer temperature and pH.

Prescribed Decay Reaction Stoichiometry. For scenarios involving chained decay reactions, EPACMTP assumes that the reaction stoichiometry is always prescribed, and the speciation factors are specified by the user as constants (see *EPACMTP Background Document,* EPA, 1993a). In reality, these coefficients may change as functions of aquifer conditions (temperature, pH, etc.) and/ or concentration levels of other chemical components.

Uniform Soil. EPACMTP assumes that the unsaturated zone profile is homogeneous. The model does not account for the presence of cracks and/or macropores in the soil, nor does it account for lateral soil variability. The latter condition may significantly affect the average transport behavior when the waste source covers a large area.

Steady-State Flow in the Unsaturated-Zone. Flow in the unsaturated zone is always treated as steady state, with the flow rate determined by the long term, average infiltration rate through a disposal unit, or by the average depth of ponding in a surface impoundment. Considering the time scale of most practical problems, assuming steady-state flow conditions in the unsaturated zone is reasonable.

Groundwater Mounding. The saturated zone module of EPACMTP is designed to simulate flow and transport in an unconfined aquifer. Groundwater mounding beneath the source is represented only by increased head values on top of the aquifer. The saturated thickness of the aquifer remains constant in the model, and therefore the model treats the aquifer as a confined system. This approach is reasonable as long as the mound height is small relative to the saturated thickness of the aquifer and the thickness of the unsaturated zone. For composite modeling, the effect of mounding is partly accounted for in the unsaturated zone module, since the soil is allowed to become saturated. The aquifer porous material is assumed to be uniform, although the model does account for anisotropy in the hydraulic conductivity. The lower aquifer boundary is assumed to be impermeable.

Flow in the Saturated Zone. Flow in the saturated zone is taken to be at steady state. The concept is that of regional flow in the horizontal longitudinal direction, with vertical disturbance due to recharge and infiltration from the overlying unsaturated zone and waste site (source area). EPACMTP accounts for variable recharge rates underneath and outside the source area. It is, however, assumed that the saturated zone has a constant thickness, which may cause inaccuracies in the predicted groundwater flow and contaminant transport in cases where the infiltration rate from the waste disposal facility is high.

Transport in the Saturated Zone. Contaminant transport in the saturated zone is by advection and dispersion. The aquifer is assumed to be initially contaminant free and contaminants enter the aquifer only from the unsaturated zone immediately underneath the waste site, which is modeled as a rectangular horizontal plane source. EPACMTP can simulate both steady state and transient transport in the saturated zone. In the former case, the contaminant mass flux entering at the water table must be constant with time. In the latter case, the flux at the water table can be constant or vary as a function of time. The transport module accounts for equilibrium adsorption and decay reactions, both of which are modeled in the same manner as in the unsaturated zone. The adsorption and decay coefficients are assumed to be uniform throughout saturated zone.

2.3 Monte Carlo Module

EPACMTP was designed to perform simulations on a nationwide basis, and to account for variations of model input parameters reflecting variations in site and hydrogeological conditions. The fate and transport model is therefore linked to a Monte Carlo driver which generates model input parameter values from the probability distribution of each parameter. The Monte Carlo modeling procedure is described in more detail in this section.

The Monte Carlo method requires that for each input parameter, except constant parameters, a probability distribution is provided. The method involves the repeated generation of pseudo-random values of the uncertain input variable(s) (drawn from the known distribution and within the range of any imposed bounds) and the application of the model using these values to generate a series of model responses (receptor well concentration). These responses are then statistically analyzed to yield the cumulative probability distribution of the model output. Thus, the various steps involved in the application of the Monte Carlo simulation technique are:

(1) Selection of representative cumulative probability distribution functions for the relevant input variables.

(2) Generation of a pseudo-random number from the distributions selected in (1). These values represent a possible set of values (a realization) for the input variables.

(3) Application of the fate and transport simulation modules to compute the output(s), i.e., downstream well concentration.

(4) Repeated application of steps (2) and (3) for a specified number of iterations.

(5) Presentation of the series of output (random) values generated in step (3).

(6) Analysis of the Monte Carlo output to derive regulatory DAF values.

The Monte Carlo module designed for implementation with the EPACMTP composite model performs steps 2-5 above. This process is shown conceptually in Figure 2. Step 6 is performed as a post-processing step. This last step simply involves converting the normalized receptor well concentrations to DAF values, and ranking then for high to low values. Each Monte Carlo iteration yields one DAF value for the constituent of concern (plus one DAF value for each of the transformation products, if the constituent is a degrader). Since each Monte Carlo iteration has equal probability, ordering the DAF values from high to low, directly yields their cumulative probability distribution (CDF). If appropriate, CDF curves representing different regional distributions may be combined into a single CDF curve, which is a weighted average of the regional curves.

A simplified flow chart that illustrated the linking of the Monte Carlo module to the simulation modules of the EPACMTP composite model is presented in Figure 3. The modeling input data is read first, and subsequently the desired random numbers are generated. The generated random and/ or derived parameter values are then assigned to the model variables. Following this, the contaminant transport fate and transport simulation is performed. The result is given in terms of the predicted contaminant concentration(s) in a down-stream receptor well. The generation of random parameter values and fate and transport simulation is repeated as many times as desired to determine the probability distribution of down-stream well concentrations.

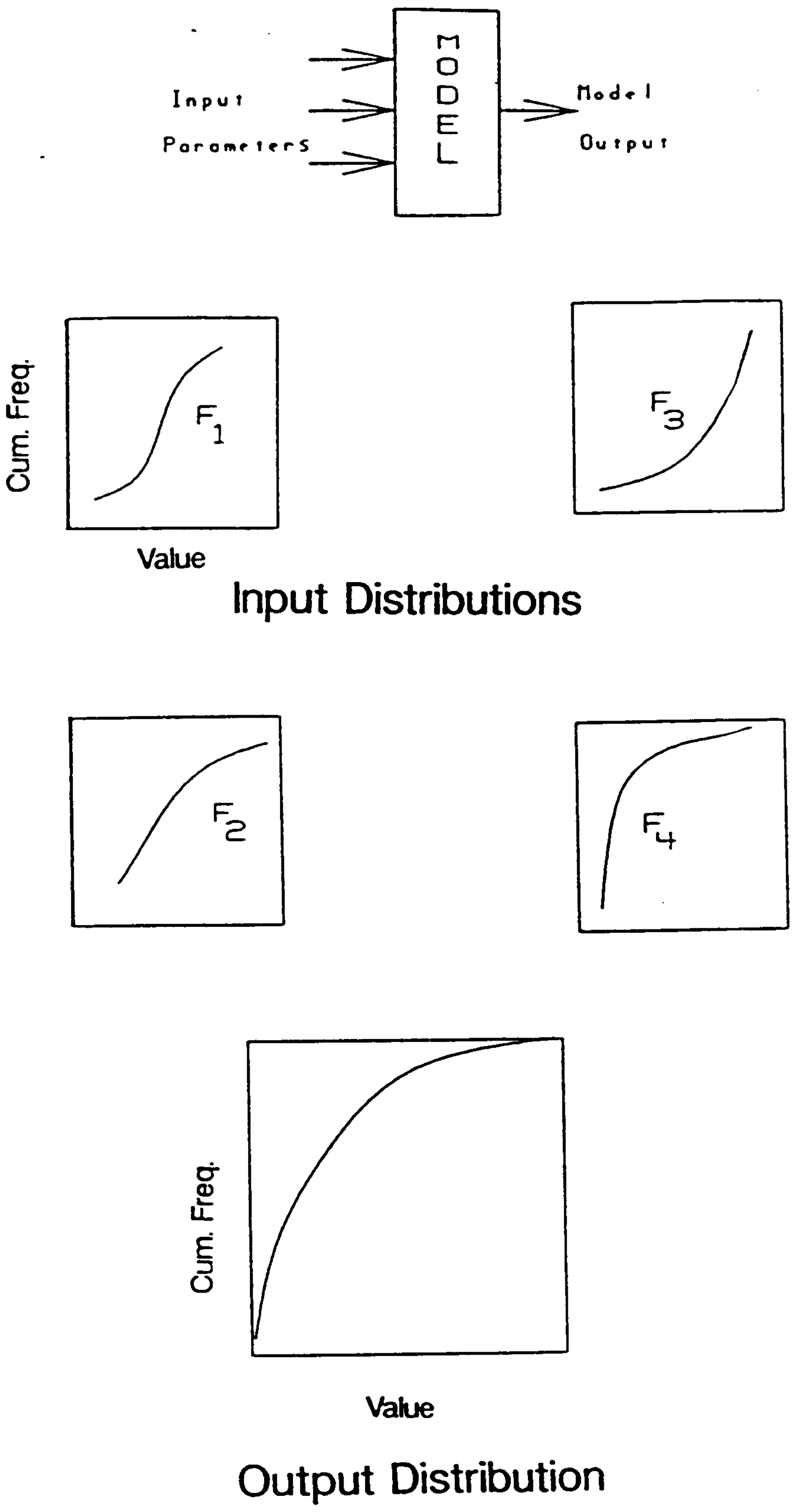


Figure 2
Conceptual Monte Carlo Framework For Deriving Probability Distribution Of Model Output From Probability Distributions Of Input Parameters

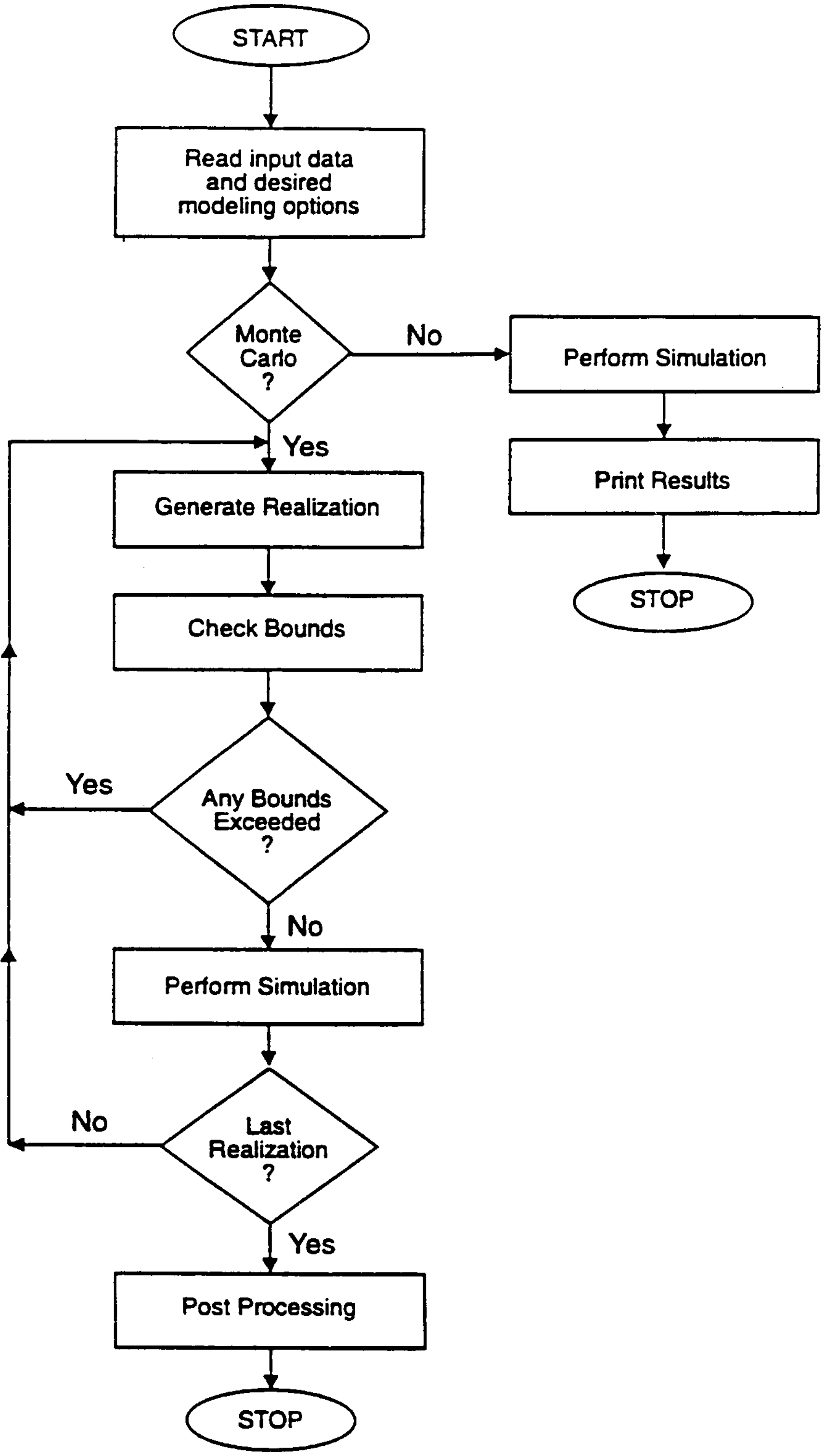


Figure 3
Flow Chart Of EPACMTP For Monte Carlo Simulation

2.3.1 Capabilities and Limitations of Monte Carlo Module

The Monte Carlo module in EPACMTP is implemented as a flexible module that can accommodate a wide variety of input distributions. These include: constant, normal, lognormal, exponential, uniform, $\log_{10}$ uniform, Johnson SB, empirical, or derived. In addition, specific upper and/or lower bounds can be provided for each parameter. The empirical distribution is used when the data does not fit any of the other probability distributions. When the empirical distribution is used, the probability distribution is specified in tabular form as a list of parameter values versus cumulative probability, from zero to one.

It is important to realize that the Monte Carlo method accounts for parameter variability and uncertainty; it does, however, not provide a way to account or compensate for process uncertainty. If the actual flow and transport processes that may occur at different sites, are different from those simulated in the fate and transport module, the result of a Monte Carlo analysis may not accurately reflect the actual variation in groundwater concentrations.

EPACMTP does not directly account for potential statistical dependencies, i.e., correlations between parameters. The probability distributions of individual parameters are considered to be statistically independent. At the same time, EPACMTP does incorporate a number of safeguards against generating impossible combinations of model parameters. Lower and upper bounds on the parameters prevent unrealistically low or high values from being generated at all.

In the case of model parameters that have a direct physical dependence on other parameters, these parameters can be specified as derived parameters. For instance, the ambient groundwater flow rate is determined by the regional hydraulic gradient and the aquifer hydraulic conductivity. In the Monte Carlo analyses, the ambient groundwater flow rate is therefore calculated as the product of conductivity and gradient, rather than generated independently. A detailed discussion of the derived parameters used in the model is provided in the *EPACMTP User's Guide* (EPA, 1994).

3.0 MODELING PROCEDURE

This section documents the modeling procedure followed in determining the groundwater pathway DAF values for the Soil Screening Levels. Section 3.1 describes the overall approach for the modeling analysis; section 3.2 describes the model options used and summarizes the input parameter values.

3.1 Modeling Approach

The overall modeling approach consisted of two stages. First, a sensitivity analysis was performed to determine the optimal number of Monte Carlo repetitions required to achieve a stable and converged result, and to determine which site-related parameters have the greatest impact on the DAFs. Secondly, Monte Carlo analyses were performed to determined DAF values as a function of the size of the source area, for various scenarios of receptor well placement.

3.1.1 Determination of Monte Carlo Repetition Number and Sensitivity Analysis

The criterion for determining the optimal number of Monte Carlo repetitions was set to a change in DAF value of no more than 5 percent when the number of repetitions is varied. A Monte Carlo simulation comprising 20,000 repetitions was first made. The results from this simulation were analyzed by calculating the 85th percentile DAP value obtained by sampling model output sequences of different length, from 2,000 to the full 20,000 repetitions. The modeling scenario considered in this analysis was the same as that in the base case scenario discussed in the next section, with the size of the source area set to 10,000 m^2.

The sensitivity analysis on site-related model parameters was performed by fixing one parameter at a time, while remaining model parameters were varied according to their default, nationwide probability distributions as discussed in the *EPACMTP User's Guide* (EPA, 1993b).

For each parameter, the low, medium, and high values were selected, corresponding to the 15th, 50th, and 85th percentile, respectively, of that parameter's probability distribution. As a result, the sensitivity analysis reflects, in part, the width of each parameter's probability distribution. Parameters with a narrow range of variation will tend to be among the less sensitive parameters, and vice versa for parameters that have a wide range of variation. By conducting the sensitivity analysis as a series of Monte Carlo simulations, any parameter interactions on the model output are automatically accounted for. Each of the Monte Carlo simulations yields a probability distribution of predicted receptor well concentrations. Evaluating the distributions obtained with different fixed values of the same parameter provides a measure of the overall sensitivity and impact of that parameter. In each case the model was run for 2,000 Monte Carlo iterations. Steady-state conditions (continuous source) were simulated in all cases.

In a complete Monte Carlo analysis, over 20 different model parameters are involved. These parameters may be divided into two broad categories. The first includes parameters that are independent of contaminant-specific chemical properties, e.g., depth to water table, aquifer thickness, receptor well distance, etc. The second category encompasses those parameters that are related to contaminant-specific sorption and biochemical transformation characteristics. This category includes the organic carbon partition coefficient, but also parameters such as aquifer pH, temperature and fraction organic carbon. The sensitivity of the model to the first category of parameters has examined, by considering a non-degrading, non-sorbing contaminant. Under these conditions, any parameters in the second category will have zero sensitivity. In addition, all unsaturated zone parameters can be left out of the analysis, since the predicted steady state contaminant concentration at the water table will always be the same as that entering the unsaturated zone. The only exception to this is the soil type parameter. In the nationwide Monte Carlo modeling approach, different soil types are distinguished. Each of the three different soil types (sandy loam, silt loam or silty clay loam) has a different distribution of infiltration rate, with the sandy loam soil type having the highest infiltration rates, silty clay loam having the lowest, and silty loam having intermediate rates. The effect of the soil type parameter is thus intermixed with that of infiltration rate. Table 1 lists the input 'low', 'medium' and 'high' values for all the parameters examined.

Table 1
Parameter input values for model sensitivity analysis.

Parameter	Low	Median	High
Source Parameters			
Source Area (m^2)	$4.8x10^4$	$2.8x 10^5$	$1.1 x10^6$
Infiltration Rate (m/yr)	$6.0x10^{-4}$	$6.4x10^{-3}$	$1.7x10^{-1}$
Recharge Rate (m/yr)	$6.0x10^{-4}$	$8.0x10^{-3}$	$1.5x10^{-1}$
Saturated Zone Parameters			
Saturated Thickness (m)	15.55	60.8	159.3
Hydraulic conductivity (m/yr)	$1.9 x 10^3$	$1.5 x 10^4$	$5.5 X 10^4$
Regional gradient	$4.3 x 10^{-3}$	$1.8 x 10^{-2}$	$5.0 X 10^{-2}$
Ambient groundwater velocity (m/yr)	53.2	404.0	2883.0
Porosity	0.374	0.415	0.455
Longitudinal Dispersivity (m)	4.2	12.7	98.5
Transverse Dispersivity (m)	0.53	1.59	12.31
Vertical Dispersivity (m)	0.026	0.079	0.62

3.1.2 Analysis of DAF Values for Different Source Areas

Following completion of the sensitivity analysis discussed above, an analysis was performed of the variation of DAF values with size of the contaminated area. The sensitivity analysis, results of which are presented in Section 4.1, showed that the size of the contaminated source area is one of the most sensitive parameters in the model. For the purpose of deriving DAF values for the groundwater pathway in determining soil screening levels, it would therefore be appropriate to correlate the DAF value to the size of the contaminated area.

The EPACMTP modeling analysis was designed to determine the size of the contaminated area that would result in DAF values of 10 and 100 at the upper 85th, 90th, and 95th percentile of probability, respectively. Since it is not possible to directly determine the source area that results in a specific DAF value, the model was executed for a range of different source areas, using a different but fixed source area value in each Monte Carlo simulation. The 85th, 90th, and 95th percentile DAF values were then plotted against source area, in order to determine the value of source area corresponding to a specific DAF value.

3.1.2.1 *Model Options and Input Parameters*

Table 2 summarizes the EPACMTP model options used in performing the simulations. Model input parameters used are summarized in Table 3. The selected options and input parameter distributions and values are consistent with those used in the default nationwide modeling, and are discussed individually in the *EPACMTP User's Guide (EPA*, 1994). Exceptions to this default modeling scenario are discussed below.

Table 2
Summary of EPACMTP modeling options.

Option	Value Selected
Simulation Type	Monte Carlo
Number of Repetitions	15,000
Nationwide Aggregation	Yes
Source Type	Continuous
Unsat. Zone Present	Yes
Sat. Zone Model	Quasi-3D
Contaminant Degradation	No
Contaminant Sorption	No

Source Area

In the default, nationwide modeling scenario, the waste site area, or source area, is treated as a Monte Carlo variable, with a distribution of values equal to that of the type of waste unit, e.g. landfills, considered. In the present modeling analyses, the source area was set to a different but constant value in each simulation run.

Receptor Well Location

In the default nationwide modeling scenario, the position of the nearest downgradient receptor well in the saturated zone is treated as a Monte Carlo variable. The position of the well is defined by its x-, y-, and z-coordinates. The x-coordinate represents the distance along the ambient groundwater flow direction from the downgradient edge of the contaminated area. The y-coordinate represents the horizontal transverse distance of the well from the plume centerline. The x-, and y-coordinate in turn can be defined in terms of an overall downgradient distance, and an angle off-center (EPA, 1994). The z-coordinate represents the depth of the well intake point below the water table. This is illustrated schematically in Figure 4, which shows the receptor well location in both plan view and cross-sectional view.

In the default nationwide modeling scenario, the x-, and z-coordinates of the well are determined from Agency surveys on the distance of residential wells from municipal landfills, and data on the depth of residential drinking water wells, respectively. The y-coordinate value is determined so that the well location falls within the approximate areal extent of the contaminant plume (see Figure 4).

For the present modeling analysis, a number of different receptor well placement scenarios were considered. These scenarios are summarized in Table 4.

Table 3
Summary of EPACMTP input parameters.

Parameter	Value or Distribution Type	Comment
Source-Specific		
Area	Constant	Varied in each run
Infiltration Rate	Soil-type dependent	default
Recharge Rate	Soil-type dependent	default
Leachate Concentration	= 1.0	default
Chemical-Specific		
Hydrolysis Rate Constants	= 0.0	Contaminant does not degrade
Organic Carbon Partition Coeff.	= 0.0	Contaminant does not sorb
Unsaturated Zone Specific		
Depth to Water Table	Empirical	default
Dispersivity	Soil-depth dependent	default
Soil Hydraulic Properties	Soil-type dependent	default
Soil Chemical Properties	Soil-type dependent	default
Saturated Zone Specific		
Sat. Zone Thickness	Exponential	default
Hydraulic Conductivity	Derived from Part. Diam.	default
Hydraulic Gradient	Exponential	default
Seepage Velocity	Derived from Conductivity and Gradient	default
Particle Diameter	Empirical	default
Porosity	Derived from Part. Diam	default
Bulk Density	Derived from Porosity	default
Longitudinal Dispersivity	Distance-dependent	default
Transverse Dispersivity	Derived from Long. Dispersivity	default
Vertical Dispersivity	Derived from Long. Dispersivity	default
Receptor Well x-coordinate	= 25 feet	Set to fixed value
Receptor Well y-coordinate	Within plume	default
Receptor Well z-coordinate	Empirical	default

Note: 'Default' represents default nationwide Monte Carlo scenario as presented in *EPACMTP User's Guide* (EPA, 1994).

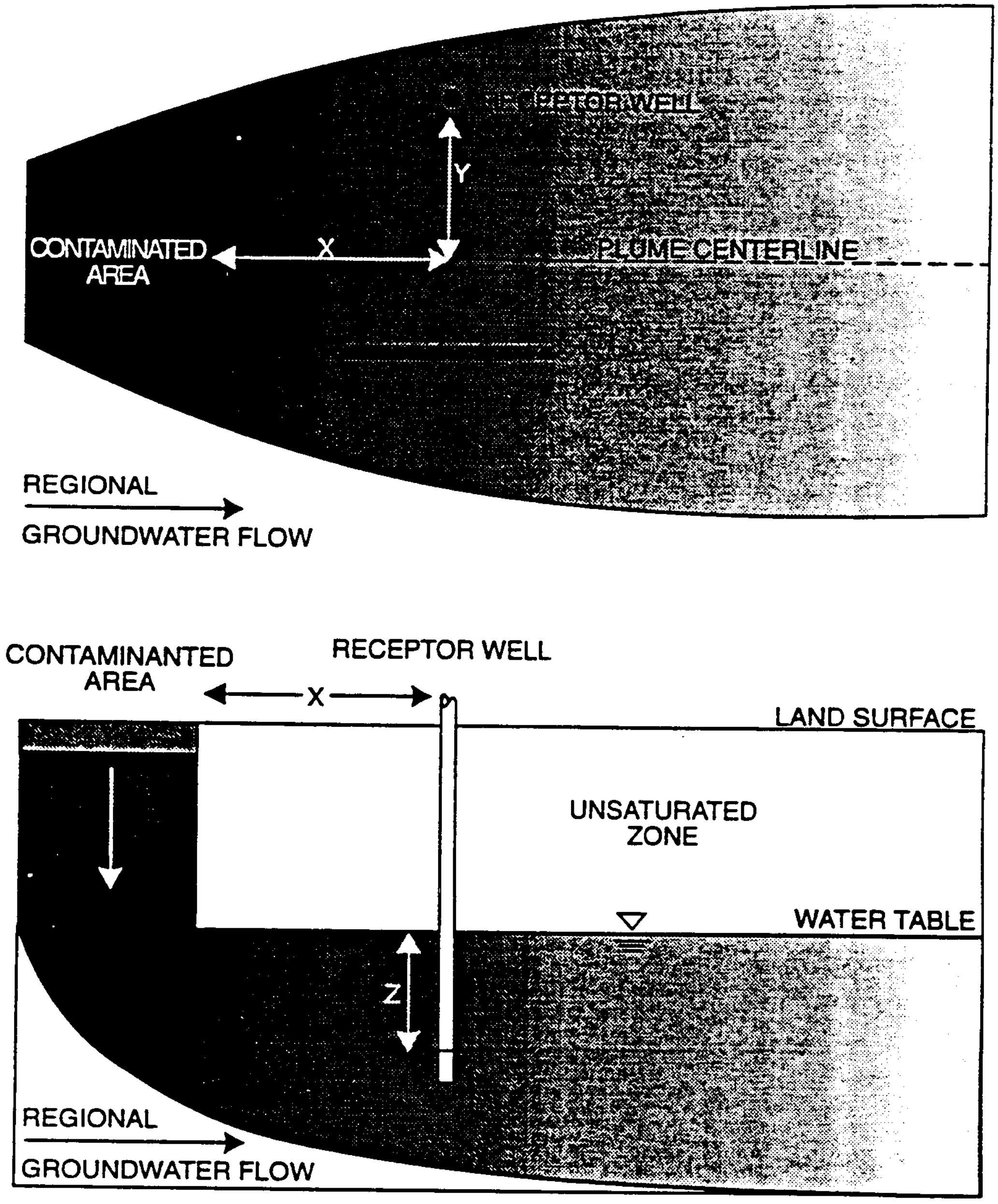


Figure 4
Plain View And Cross-Section View Showing Location Of Receptor Well

Table 4
Receptor Well Location Scenarios

Scenario	Xwell	Ywell	Zwell
1 (Base Case)	25 ft from edge of source area	Monte Carlo within plume	Nationwide Distribution
2	Nationwide Distribution	Monte Carlo within plume	Nationwide Distribution
3	0 ft from edge of source area	Monte Carlo within half-width of source area	Nationwide Distribution
4	25 ft from edge of source area	Monte Carlo within half-width of source area	Nationwide Distribution
5	100 ft from edge of source area	Monte Carlo within half-width of source area	Nationwide Distribution
6	25 ft from edge of source area	Width of source area + 25 ft	25 ft below water table

Xwell = Downgradient distance of receptor well from edge of source area.
Ywell = Horizontal transverse distance from plume centerline.
Zwell = Depth of well intake point below water tablet

The base case scenario (scenario 1) involved setting the x-distance of the receptor well to 25 feet from the edge of the source area. Nationwide default options were used for the receptor well y- and z-coordinates. The y-coordinate of the well was assigned a uniform probability distribution within the boundary of the plume. The depth of the well intake point (z-coordinate) was assumed to vary within upper and lower bounds of 15 and 300 feet below the water table, reflecting a national sample distribution of depths of residential drinking water wells (EPA, 1994).

In addition to this base case scenario, a number of other well placement scenarios were investigated also. These are numbered in Table 4 as scenarios 2 through 6. Scenario 2 corresponds to the default, nationwide Monte Carlo modeling scenario in which the x, y, and z locations of the well are all variable. In scenarios 3, 4 and 5, the distance between the receptor well and the source area is varied from zero to 100 feet. In these scenarios, the ycoordinate of the well was constrained to the central portion of the plume. In scenario number 6, the x-, y-, and z-coordinates of the receptor well were all set to constant values. These additional scenarios were included in the analysis in order to assess the sensitivity of the model results to the location of the receptor well.

Aquifer Particle Size Distribution

In the default Monte Carlo modeling scenario, the aquifer hydraulic conductivity, porosity, and bulk density are determined from the mean particle diameter. The particle diameter distribution used is based on data compiled by Shea (1974). In the present modeling analyses for fixed waste site areas, the same approach and data were used, but the distribution was shifted somewhat to assign more weight to the smallest particle diameter interval. The result is that lower values of the hydraulic conductivity values generated, and also of the ambient groundwater seepage velocities, received more emphasis. Lower ambient groundwater velocities reduce the degree of dilution of the incoming contaminant plume and therefore result in lower, i.e. more conservative, DAF values. Table 5 summarizes the distribution of particle size diameters used in both the default nationwide modeling scenario and in the present analyses.

Table 5
Distribution of aquifer particle diameter.

Nationwide Default		Present Analyses	
Particle Diameter (cm)	**Cumulative Probability**	**Particle Diameter (cm)**	**Cumulative Probability**
3.9 10^{-4}	0.000	4.0 10^{-4}	0.100
7.8 10^{-4}	0.038	8.0 10^{-4}	0.150
1.6 10^{-3}	0.104	1.6 10^{-3}	0.200
3.1 10^{-3}	0.171	3.1 10^{-3}	0.270
6.3 10^{-3}	0.262	6.3 10^{-3}	0.330
1.25 10^{-2}	0.371	1.25 10^{-2}	0.440
2.5 10^{-2}	0.560	2.5 10^{-2}	0.590
5.0 10^{-2}	0.792	5.0 10^{-2}	0.790
1.0 10^{-1}	0.904	1.0 10^{-1}	0.880
2.0 10^{-1}	0.944	2.0 10^{-1}	0.910
4.0 10^{-1}	0.946	4.0 10^{-1}	0.940
8.0 10^{-1}	1.000	7.5 10^{-1}	1.000

4.0 RESULTS

This section presents the results of the modeling analyses performed. The analysis of the convergence of the Monte Carlo simulation is presented first, followed by the parameter sensitivity analysis, and thirdly the analysis of DAF values as a function of source area for various well placement scenarios.

4.1 Convergence of Monte Carlo Simulation

Table 6 summarizes the results of this convergence analysis. It shows the variation of the 85th percentile DAF value with the number of Monte Carlo repetitions, from 2,000 to 20,000. The variations in DAF values are shown both as absolute and relative differences. The table shows that for this example, the DAF generally increases with the number of Monte Carlo repetitions. It should be kept in mind that the results from different repetition numbers as presented in the table, are not independent of one another. For instance, the first 2,000 repetitions are also incorporated in the 5000 repetition results, which in turn is in the 10,000 repetition result, etc. The rightmost column of Table 6 shows the percentage difference in DAF value between different repetition numbers. At repetition numbers of 14,000 or less, the percentage difference varies in a somewhat irregular manner. However, for repetition numbers of 15,000 or greater, the DAF remained relatively constant, with incremental changes of DAF remaining at 1 % or less. Based upon these results, a repetition number of 15,000 was selected for use in the subsequent runs with fixed source area.

4.2 Parameter Sensitivity Analysis

Results of the parameter sensitivity analysis are summarized in Table 7. The parameters are ranked in this table in order of relative sensitivity. Relative sensitivity is defined for this purpose as the absolute difference between the "high" and "low" DAF at the 85th percentile level, divided by the 85th percentile DAF for the "median" case.

The table shows that the most sensitive parameters included the rate of infiltration, which is a function of soil type, the saturated thickness of the aquifer, the size of source area, the groundwater seepage velocity, and the vertical position of the receptor well below the water table. The least sensitive parameters included porosity, downstream distance of the receptor well in both the x- and y-directions, the horizontal transverse dispersivity, and the areal recharge rate. To interpret these results, it should be kept in mind that the rankings reflect in part the range of variation of each parameter in the data set used for the sensitivity analysis. The infiltration rate was a highly sensitive parameter since, for a given leachate concentration, it directly affects the mass flux of contaminant entering the subsurface. The size of the source would be expected to be equally sensitive, were it not for the fact that in the sensitivity analysis, the source area had a much narrower range of variation than the infiltration rate. The "high" and "low" values of the source area, which were taken from a nationwide distribution of landfill waste units, varied by a factor of 23, while the ratio of "high" to "low" infiltration rate was almost 300.

In the simulations performed for the sensitivity analysis, no constraint was imposed on the vertical position of the well. The well was modeled as having a uniform distribution with the well intake point located anywhere between the water table and the base of the aquifer. The aquifer saturated thickness and vertical position of the well were both among the sensitive parameters, with similar effects on DAF values. Increasing either the saturated thickness, or the fractional depth of the receptor well below the water table, increases the likelihood that the receptor well will be located underneath the contaminant plume and sample uncontaminated groundwater, leading to a

Table 6
Variation of DAF with number of Monte Carlo repetitions

No. of Repetitions	85-th Percentile DAF	Difference	Relative Difference (%)
2,000	347.8		
		-10.9	-3.1
5,000	336.9		
		+17.3	+5.1
10,000	354.2		
		+5.0	+ 1.4
11,000	359.2		
		+28.2	+7.9
12,000	387.4		
		-18.1	-4.7
13,000	369.3		
		-0.2	-0.05
14,000	369.1		
		+ 18.2	+4.9
15,000	387.3		
		+0.1	+0.03
16,000	387.4		
		+0.6	+0.15
17,000	388.0		
		-0.7	-0.18
18,000	387.3		
		+2.9	+0.75
19,000	390.2		
		+2.6	+0.67
20,000	392.8		

Table 7
Sensitivity of model parameters.

Parameter	85% DAF Value			Relative Sensitivity*	Rank
	Low	Median	High		
Infiltration Rate	4805.4	418.8	11.6	11.4	1
Saturated Thickness	25.3	198.5	2096.9	10.4	2
G.W. Velocity	7.6	97.7	816.3	8.3	3
Source Area	357.1	85.2	35.6	3.8	4
Hydr. Conductivity	19.8	180.4	660.1	3.5	5
Vertical Well Position	49.1	206.1	491.4	2.1	6
G.W. Gradient	32.4	168.3	383.0	2.1	7
Long. Dispersivity	182.6	104.2	78.8	1.0	8
Vert. Dispersivity	179.6	114.9	66.6	1.0	9
Porosity	41.3	49.9	79.7	0.8	10
Receptor Well Distance	163.9	117.9	84.5	0.7	11
Transv. Dispersivity	156.7	156.3	173.5	0.1	12
Receptor Well Angle	127.3	130.8	113.6	0.1	13
Ambient Recharge	108.3	100.0	114.4	0.06	14

* Relative Sensitivity = l High-Low l /Median

high DAF value. The dilution-attenuation factors were also sensitive to the groundwater velocity, and the parameters that determine the groundwater velocity, i.e., hydraulic conductivity and ambient gradient. Table 7 shows that a higher groundwater velocity results in an increase of the dilution-attenuation factor. Since a conservative contaminant was simulated under steady-state conditions, variations in travel time do not affect the DAF. The increase of DAF with increasing flow velocity reflects the greater mixing and dilution of the contaminant as it enters the saturated zone in systems with high groundwater flow rate. Porosity also directly affects the groundwater velocity, but was not among the sensitive parameters. This is a reflection of the narrow range of variation assigned to this parameter.

The off-center angle which determines the y position of the well relative to the plume center line would be expected to have a similar effect as the well depth, but is seen to have a much smaller sensitivity. This was a result of constraining the y-location of the receptor well to be always inside the approximate areal extent of the contaminant plume. The effect is that the relative sensitivity of the off-center angle was much less than that of the vertical coordinate of the well. The low relative sensitivity of recharge rate reflects the fact that this parameter has an only indirect effect on plume concentrations.

Overall, the Monte Carlo results were not very sensitive to dispersivity and downstream distance of the receptor well. The probable explanation for these parameters is that variations of the parameters produce opposing effects which tended to cancel one another. Low dispersivity values will produce a compact plume which increases the probability that a randomly located receptor well will lie outside (underneath) the plume. Higher dispersivities will increase the chance that the well will intercept the plume. At the same time, however, mass balance considerations dictate that in this case average concentrations inside the plume will be lower than in the low dispersivity case. Similar reasoning applies to the effect of receptor well distance. If the well is located near the source, concentrations in the plume will be relatively high, but so is the chance that the well does not intercept the plume at all. At greater distances from the source, the likelihood that the well is located inside the plume is greater, but the plume will also be more diluted. In the course of a full Monte Carlo simulation these opposing effects would tend to average out. The much lower sensitivity of transverse dispersivity, α_T, compared to α_L and α_V can be contributed to the imposed constraint that the well must always be within the areal extent of the plume.

The results of the sensitivity analysis show that the site characteristic which lends itself best for a classification system for correlating sites to DAF values is the size of the contaminated (or source) area. In the subsequent analyses, the DAF values were therefore determined as a function of the source area size. These results are presented in the following section.

4.3 DAF Values as a Function of Source Area

This section presents the DAF value as a function of source area for various well location scenarios. The results for each of the scenarios examined are presented in tabular and graphical form. Figure 5 shows the variation of the 85th, 90th, and 95th percentile DAF with source area for the base case scenario. The source area is expressed in square feet. The figure displays DAF against source area in a log-log graph. The graph shows an approximately linear relationship except that at very large values of the source area, the DAF starts to level off. Eventually the DAF approaches a value of 1.0. As expected, the curve for the 95th percentile DAF always shows the lowest DAF values, while the 85th percentile shows the highest DAFs. The DAF versus source area relationship for the other well placement scenarios are shown in Figures 6 through 10. The numerical results for each scenario are summarized in Tables Al through A6 in the appendix.

Inspection and comparison of the results for each scenario indicate that the relationship follows the same general shape in each case, but the magnitude of DAF values at a given source area can be quite different for different well placement scenarios. In order to allow a direct comparison between the various scenarios analyzed, the DAF values obtained for a source area of 150,000 ft^2 (3.4 acres) are shown in Table 8 as a function of the receptor well location scenario.

Inspection of the DAF values shows that the default nationwide scenario for locating the receptor well results in the highest DAF values, as compared to the base case scenario and the other scenarios, in which the receptor well location was fixed at a relatively close distance from the waste source. In the default nationwide modeling scenario, the well location is assigned from nationwide data on both the distance from the waste source and depth of the well intake point below the water table. In the default nationwide modeling scenario, the receptor well is allowed to be located up to 1 mile from the waste source. In the base case (Scenario 1) the well is allowed to be located anywhere within the areal extent of the contaminant plume for a fixed x-distance of 25 feet. This allows the well to be located near the fringes of the contaminant plume where concentrations are relatively low and DAF values are correspondingly high. In contrast, in Scenarios 3, 4, and 5, the well location was constrained to be within the half-width of the waste source. In other words, the well was always placed in the central portion of the contaminant plume where concentrations are highest. As a result, these scenarios show lower DAF values then the base case scenario. The results for Scenarios 3, 4, and 5, which differ only in the x-distance of the receptor well, show that placement of the well at either 25 or 100 feet away from the waste source results in 85% and 90% DAF values that are actually lower, i.e. more conservative, than placement of the well directly at the edge of the waste source. This is a counter-intuitive result, but may be explained from the interaction between distance from the waste source and vertical extent of the contaminant plume below the water table. Close to the waste source, the contaminant concentrations within the plume are highest, but the plume may not have penetrated very deeply into the saturated zone (Figure 2).

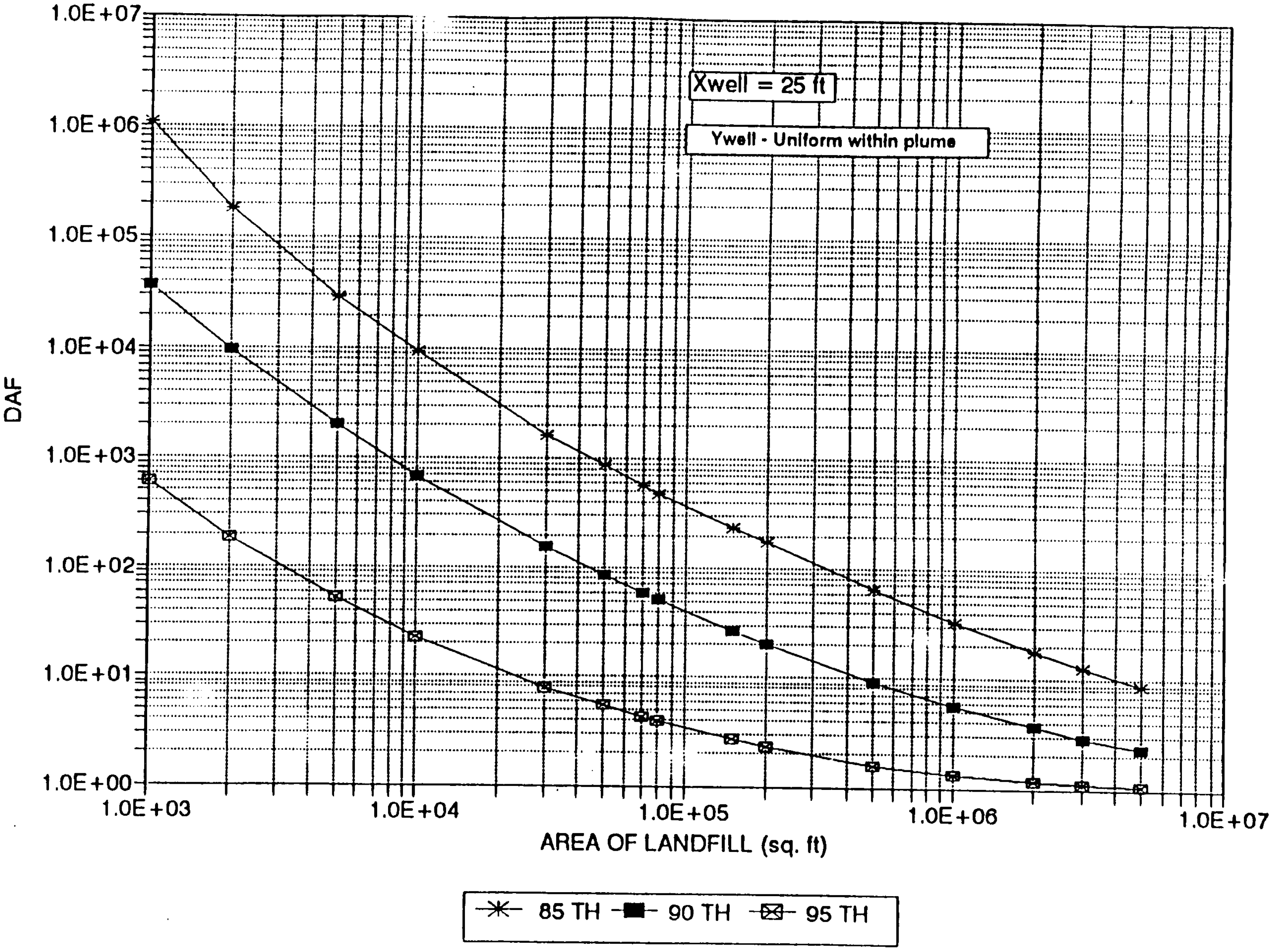


Figure 5
Variation Of DAF With Size Of Source For The Base Case Scenario (x=25 ft, y=uniform in plume, z=nationwide distribution)

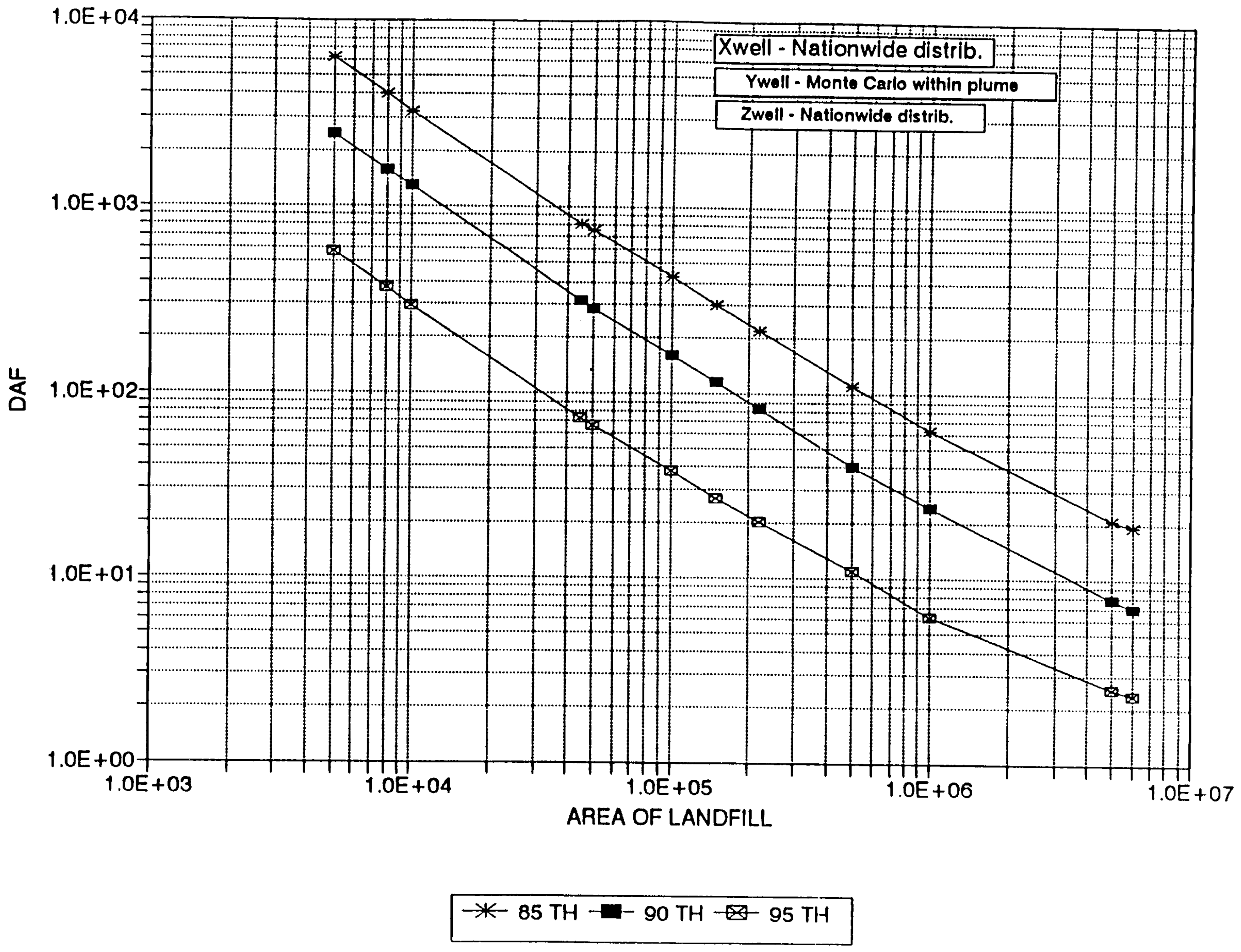


Figure 6
Variation Of DAF With Size Of Source Area For The Default Nationwided Scenario
(Scenario 2: x=nationwide distribution, y=uniform in plume, z=nationwide distribution)

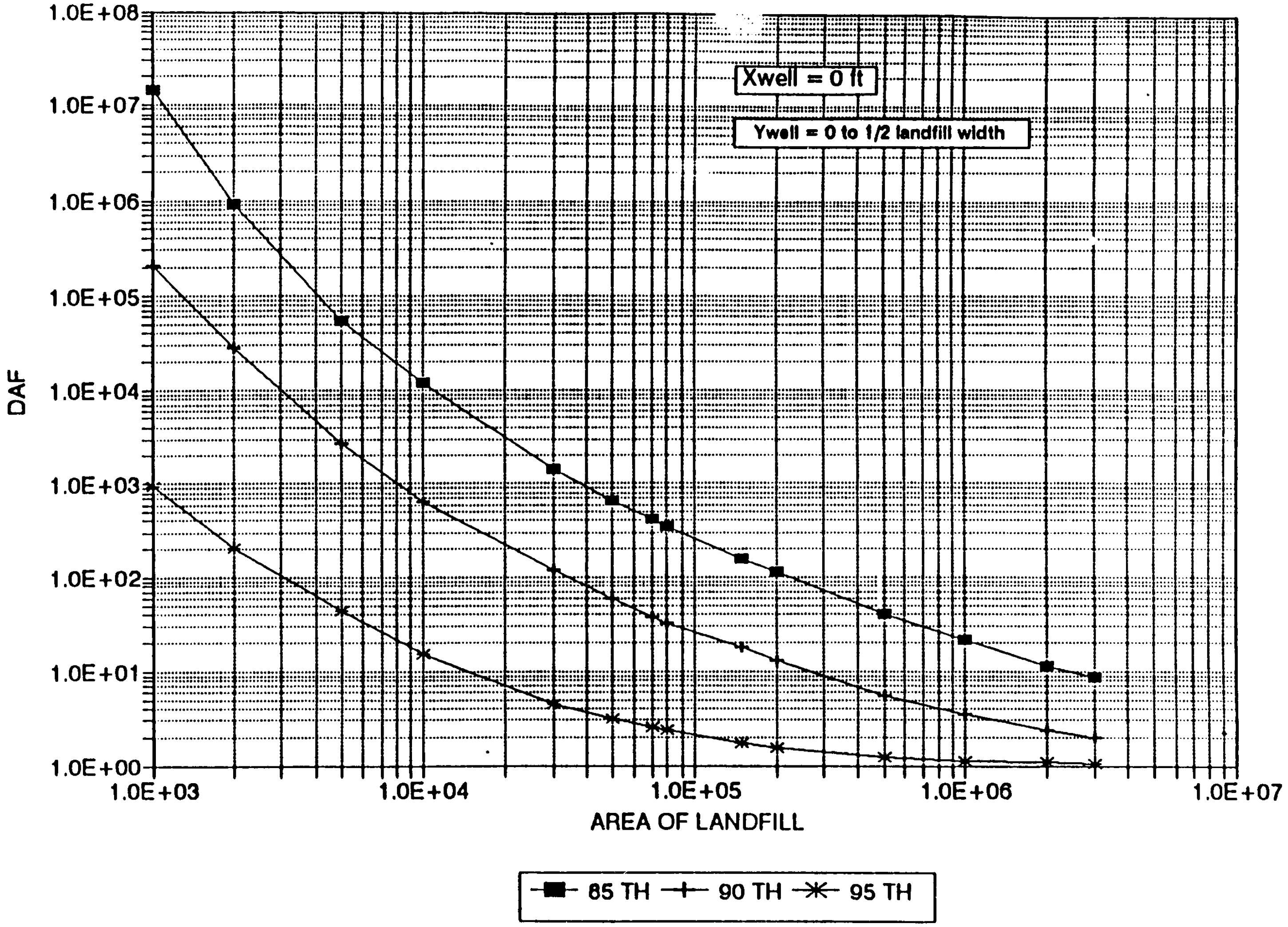


Figure 7
Variation Of DAF With Size Of Source Area For Scenario 3
(x=0, y=uniform within half-width of source area, z=nationwide distribution

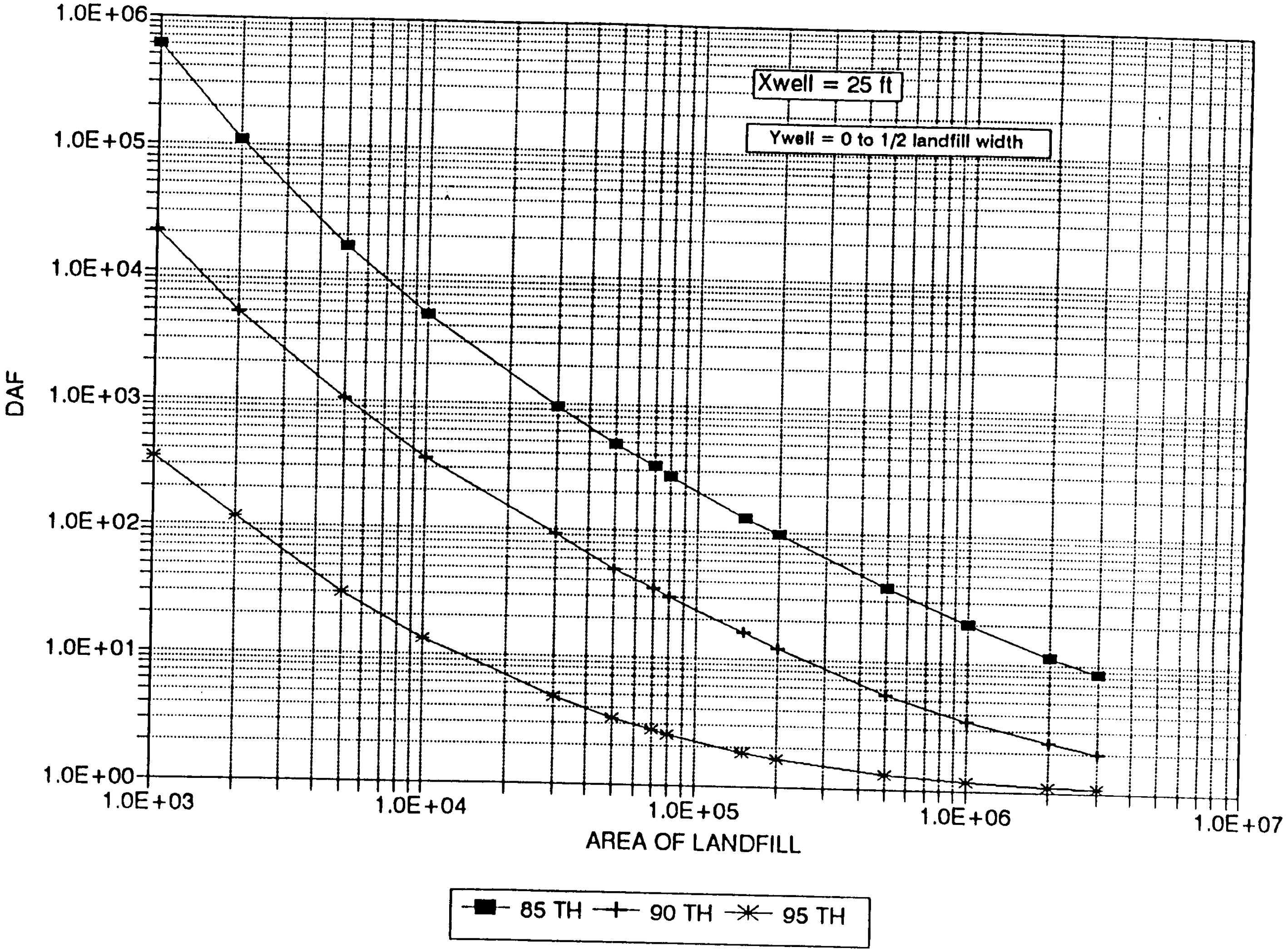


Figure 8
Variation Of DAF With Size Of Source Area For Scenario 4
(x=25 fy, y=uniform within half-width of source area, z=nationwide distribution)

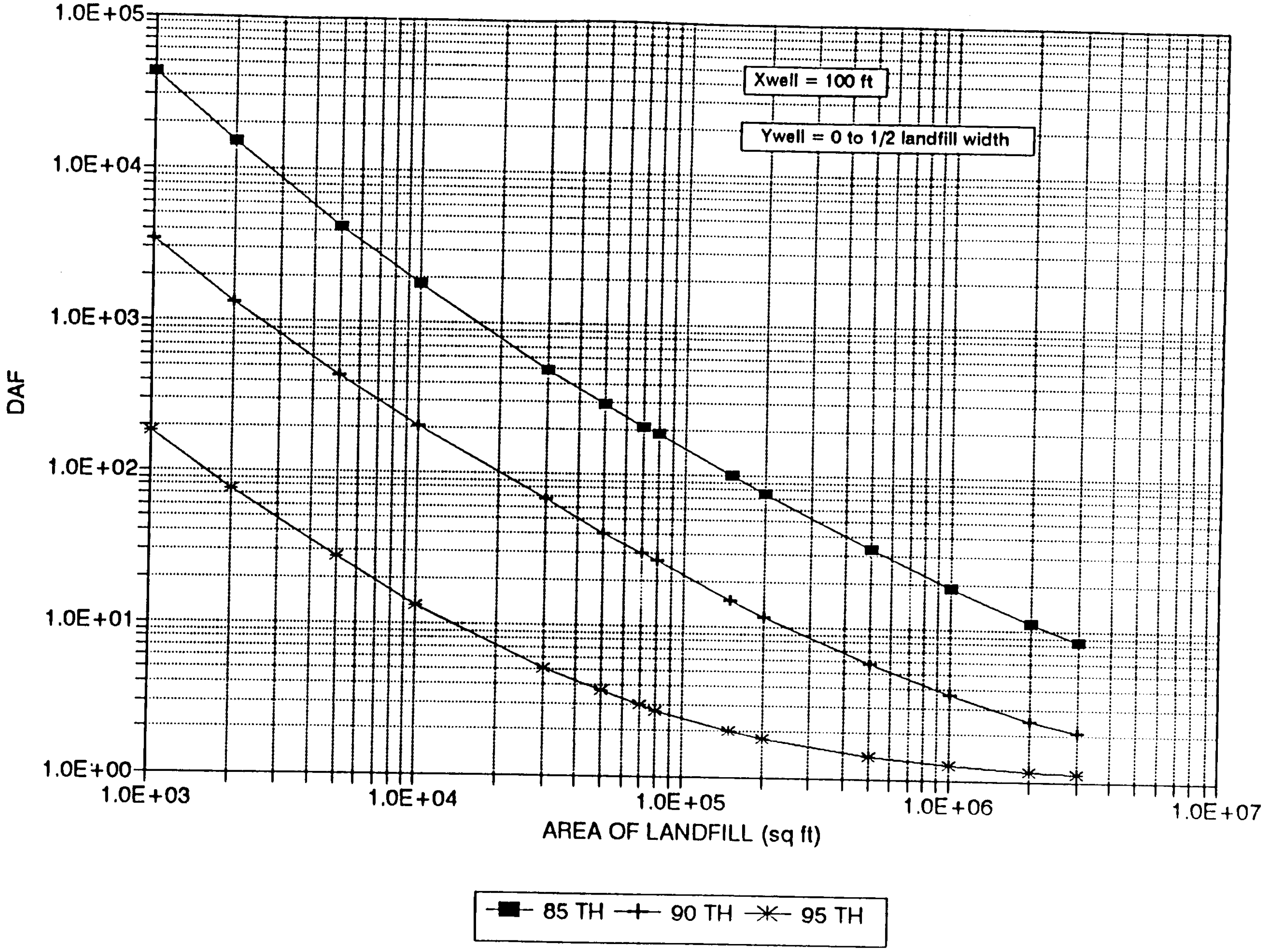


Figure 9
Variation Of DAF With Size Of Source Area For Scenario 5
(x=100 ft, y=uniform within half-width of source area, z=nationwide distribution)

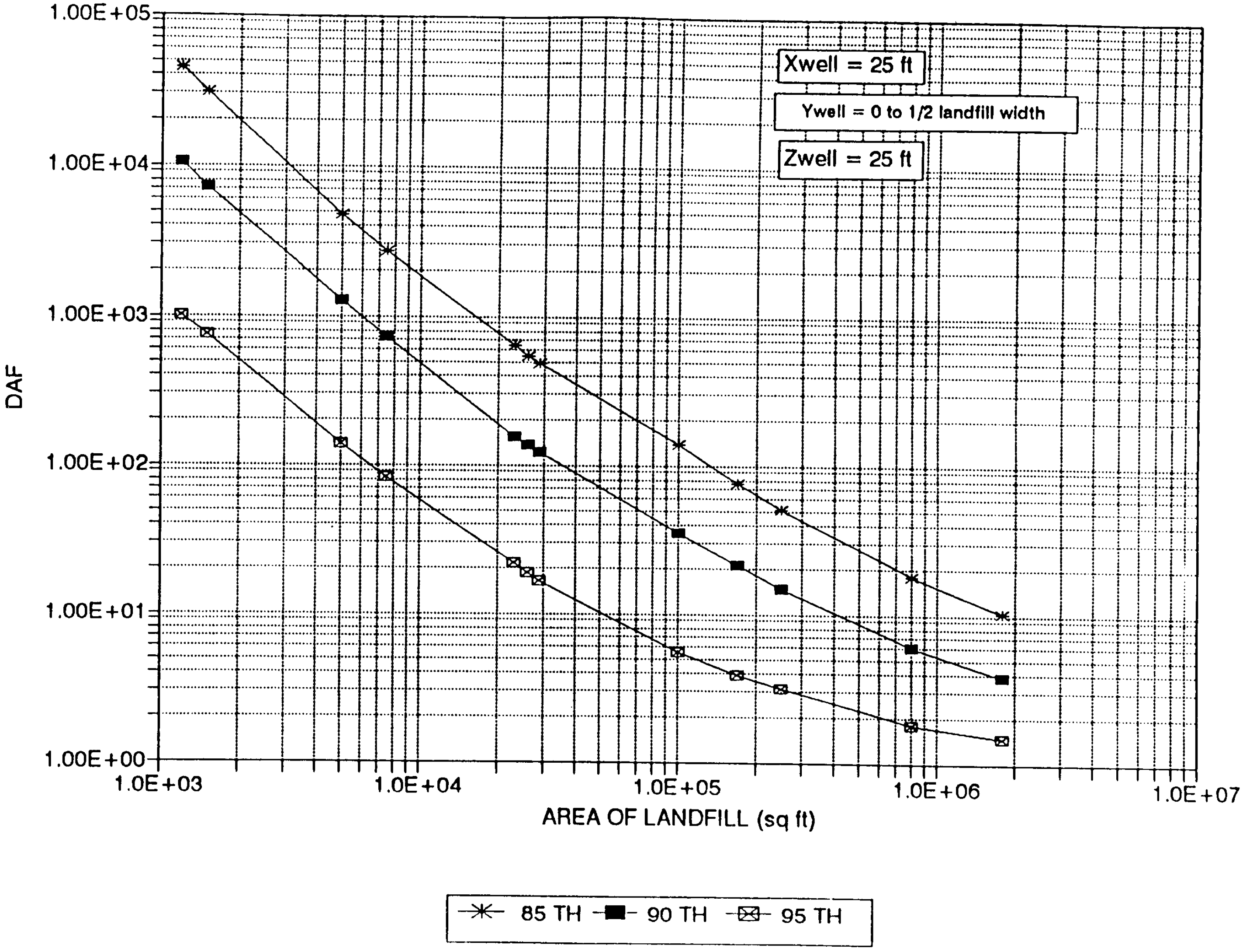


Figure 10
Variation Of DAF With Size Of Source Area For Scenario 6
(x=25 ft, y=width of source area + 25 ft, z=25 ft)

Table 8
DAF values for waste site area of 150,000 ft^2.

	DAF Percentile		
Model Scenario	**85**	**90**	**95**
1 (base case)	237.5	26.4	2.8
2	300.1	114.7	26.8
3	158.8	17.9	1.7
4	132.1	16.6	1.8
5	98.8	15.1	2.0
6	94.7	25.3	4.4

Because the vertical position of the well was taken as a random variable, with a maximum value of up to 300 feet, the probability that a receptor well samples pristine groundwater underneath the contaminant plume is higher at close distances from the waste area. Conversely, as the distance from the source increases, the plume becomes more dilute but also extends deeper below the water table. The final result is that the overall DAF may actually decrease with distance from the source. The table also shows that at the 95% level, the lowest DAF is obtained in the case where the well is located at the edge of the waste source. This reflects that the highest concentration values will be obtained only very close to the waste source.

The results for the last scenario, in which the x, y, and z locations of the receptor well were all fixed, show that fixing the well depth at 25 feet ensures that the well is placed shallow enough that it will be located inside the plume in nearly all cases, resulting in low DAF values at the 85th and 90th percentile values. On the other hand, the well in this case is never placed immediately at the plume centerline, so that the highest concentrations sampled in this scenario are always lower than in the other scenarios. This is reflected in the higher DAF value at the 95th percentile level.

One of the key objectives of the present analyses was to determine the appropriate groundwater DAF value for a waste area of given size. For the base case scenario, the 90th percentile DAF value is on the order of 100 or higher for a waste area size of 1 acre (43,560 ft^2) and less. For waste areas of 10 acres and greater, the 90th percentile DAF is 10 or less.

REFERENCES

Shea, J.H., 1974. Deficiencies of elastic particles of certain sizes. Journal of Sedimentary Petrology, 44:905-1003.

U.S. EPA, 1993a. EPA's Composite Model for Leachate Migration with Transformation Products: EPACMTP. Volume I: Background Document. Office of Solid Waste, July 1993.

U.S. EPA, 1993b. Draft Soil Screening Level Guidance Quick Reference Fact Sheet. Office of Solid Waste and Emergency Response, September 1993.

U.S. EPA, 1994. Modeling Approach for Simulating Three-Dimensional Migration of Land and Disposal Leachate with Transformation Products and Consideration of Water-Table Mounding. Volume II: User's Guide for EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP). Office of Solid Waste, May 1994.

APPENDIX A

Table A1 DAF values as a function of source area for base case scenario (x=25 ft., y=uniform in plume, z-nationwide distribution).

Area (sq. ft.)	DAF		
	85th	90th	95th
1000	1.09E+06	3.76E+04	609.01
2000	1.86E+05	9.63E+03	187.69
5000	2.91 E+04	2.00E+03	53.02
10000	9.31 E+03	680.27	22.57
30000	1647.18	155.21	7.82
50000	869.57	84.25	5.41
70000	569.80	59.28	4.34
80000	477.33	50.56	3.97
150000	237.47	26.36	2.77
200000	174.86	20.19	2.37
500000	64.52	9.12	1.61
1000000	32.27	5.61	1.32
2000000	17.83	3.68	1.16
3000000	12.94	2.94	1.11
5000000	8.91	2.33	1.06

Table A2 DAF values as a function of source area for Scenario 2 (x=nationwide distribution, y=uniform in plume, z=nationwide distribution).

Area (sq. ft.)	DAF		
	85th	90th	95th
5000	6222.78	2425.42	565.61
8000	3977.72	1573.32	371.06
10000	3215.43	1286.01	298.78
45000	817.66	315.06	73.48
50000	745.16	288.27	67.20
100000	424.81	160.82	38.11
150000	300.12	114.71	26.82
220000	218.87	82.30	20.00
500000	110.35	40.10	10.92
1000000	63.45	23.75	6.22
5000000	21.03	7.85	2.55
6000000	19.06	7.01	2.39

Table A3 DAF values as a function of source area for Scenario 3 (x=0 ft, y=uniform within half-width of source area, z=nationwide distribution).

	DAF		
Area (sq. ft.)	85th	90th	95th
1000	1.42E+07	2.09E+05	946.07
2000	9.19E+05	2.83E+04	211.15
5000	5.54E+04	2.74E+ 03	44.23
10000	1.16E+04	644.33	15.29
30000	1.43E+03	120.42	4.48
50000	668.45	60.02	3.10
70000	417.19	37.97	2.53
80000	350.39	33.16	2.34
150000	158.76	17.87	1.74
200000	114.63	12.96	1.56
500000	40.55	5.54	1.23
1000000	21.13	3.50	1.15
2000000	11.58	2.38	1.08
3000000	8.66	1.98	1.06

Table A4 DAF values as a function of source area for Scenario 4 (x=25 ft, y=uniform within half-width of source area, z=nationwide distribution).

Area (sq. ft.)	DAF		
	85th	90th	95th
1000	5.93E + 05	2.07E + 04	348.31
2000	1.09E+05	4.92E+03	118.11
5000	1.64E + 04	1.03E + 03	29.86
10000	4.89E+03	352.49	13.14
30000	928.51	93.98	4.73
50000	490.20	49.78	3.28
70000	323.42	34.79	2.69
80000	272.85	29.82	2.47
150000	132.05	16.55	1.82
200000	97.94	12.29	1.61
500000	37.99	5.50	1.29
1000000	20.08	3.50	1.17
2000000	11.35	2.40	1.10
3000000	8.49	2.00	1.07

Table A5 DAF values as a function of source area for Scenario 5 (x=100 ft, y=uniform within half-width of source, z=nationwide distribution).

	DAF		
Area (sq. ft.)	85th	90th	95th
1000	4.24E+04	3.43E+03	181.88
2000	1.52E + 04	1.33E + 03	74.79
5000	4.24E+ 03	437.25	27.23
10000	1.81 E+03	204.29	13.09
30000	497.27	68.21	5.10
50000	293.34	40.72	3.71
70000	207.77	29.89	2.96
80000	184.57	26.86	2.73
150000	98.81	15.05	2.03
200000	74.63	11.55	1.82
500000	32.99	5.83	1.40
1000000	18.66	3.71	1.26
2000000	11.14	2.53	1.16
3000000	8.33	2.09	1.13

Table A6 DAF values as a function of source area for Scenario 6 (x=25 ft, y=source width + 25 ft, z=25 ft).

Area (sq. ft.)	DAF		
	85th	90th	95th
1200	44247.79	10479.98	1004.72
1500	30759.77	7215.01	744.05
5000	4789.27	1273.40	140.81
7500	2698.33	725.69	82.51
23000	637.76	155.16	21.82
26000	544.66	135.91	18.84
29000	482.63	121.43	16.52
100000	139.66	35.55	5.56
170000	76.69	21.24	3.94
250000	50.40	15.04	3.19
800000	18.10	6.04	1.81
1800000	10.26	3.87	1.48

APPENDIX F

Dilution Factor Modeling Results

Dilution Factor Model Results: DNAPL Sites

Source size (acres)	0.5	10	30	100	600
Source length (m)	45	201	349	636	1,559
Aquifer thickness (m)			9.1		

		Infiltration by Hyd. Region		Average GW Velocity (m/yr)		Mixing zone depth					Dilution factor				
						Site size (acres)					Site size (acres)				
Site Name	**State**	**Region**	**(m/yr)**	**Seepage**	**Darcy**	**0.5**	**10**	**30**	**100**	**600**	**0.5**	**10**	**30**	**100**	**600**
Army Creek Landfill	DE	10	0.24	5,563	1,947	5	21	37	67	165	861	370	214	118	49
Atlantic Wood Ind.	VA	10	0.24	1,261	442	5	21	37	68	166	197	85	49	27	12
AtlasTack Corp.	MA	9	0.22	3	1	10	30	46	76	174	2	1	1	1	1
Auburn Rd. Landfill	NH	9	0.22	61	21	5	23	40	72	173	12	5	4	2	2
Baird & McGuire	MA	9	0.22	61	21	5	23	40	72	173	12	5	4	2	2
Bally Groundwater	PA	6	0.15	3,204	1,121	5	21	37	67	165	793	341	197	108	45
Beacon Hts. Landfill	CT	9	0.22	15	5	6	27	44	76	174	4	2	2	1	1
Berks Sand Pit	PA	6	0.15	10	4	6	27	44	76	174	4	2	2	1	1
Brodhead Creek	PA	7	0.20	11,246	3,936	5	21	37	67	165	2,085	895	517	284	116
Brunswick Naval Air Sta.	ME	9	0.22	230	81	5	22	38	69	168	41	18	11	6	3
Cannon Eng.- Bridgewater	MA	9	0.22	3	1	11	30	46	76	174	2	1	1	1	1
Central Landfill	RI	9	0.22	223	78	5	22	38	69	168	39	17	10	6	3
Centre County Kepone	PA	6	0.15	61,189	21,416	5	21	37	67	165	15,112	6,489	3,747	2,053	839
Chas.-Geo. Reclam. Trust	MA	9	0.22	34	12	6	24	42	74	174	8	3	2	2	1
Coakley Landfill	NH	9	0.22	113	40	5	22	39	70	171	21	9	6	4	2
Craig Farm Drum	PA	6	0.15	451	158	5	21	37	68	166	113	49	29	16	7
Davis Liquid Waste	RI	9	0.22	189	66	5	22	38	69	169	34	15	9	5	3
Delaware City PVC	DE	10	0.24	223	78	5	22	38	69	169	36	16	10	6	3
Dorney Road Landfill	PA	6	0.15	1,913	670	5	21	37	67	165	474	204	118	65	27
Dover Mun. Landfill	NH	9	0.22	289	101	5	22	38	69	168	51	22	13	8	4
DuPont-Newport	DE	10	0.24	33	12	6	25	42	74	174	7	3	2	2	1
Dublin TCE Site	PA	6	0.15	32	11	5	24	41	73	173	10	4	3	2	1
Durham Meadows	CT	9	0.22	612	214	5	21	37	68	166	105	45	27	15	7
East Mt. Zion	PA	6	0.15	1,218	426	5	21	37	68	165	303	130	76	42	18
Elizabethtown Landfill	PA	6	0.15	56	20	5	23	39	71	172	16	7	4	3	2
Gallup's Quarry	CT	9	0.22	67	23	5	23	40	72	172	13	6	4	3	2
Greenwood Chemical	VA	8	0.15	3	1	10	30	46	76	174	2	1	1	1	1
Groveland Wells	MA	9	0.22	612	214	5	21	37	68	166	105	45	27	15	7
Halby Chemical Co.	DE	10	0.24	5	2	9	30	46	76	174	2	1	1	1	1
Harvey & Knott Drum	DE	10	0.24	434	152	5	22	37	68	167	69	30	18	10	5
Havertown PCP	PA	8	0.15	24	9	6	24	41	74	174	8	4	2	2	1
Heleva Landfill	PA	6	0.15	28	10	5	24	41	73	173	9	4	3	2	1
Henderson Road	PA	6	0.15	834	292	5	21	37	68	166	208	89	52	29	12
Hocomonco Pond	MA	9	0.22	1,986	695	5	21	37	68	165	336	145	84	46	20
Holton Circle	NH	9	0.22	2,809	983	5	21	37	67	165	475	204	118	65	27
Hunterstown Road	PA	6	0.15	562	197	5	21	37	68	166	141	61	35	20	9
Industri-plex	MA	9	0.22	289	101	5	22	38	69	168	51	22	13	8	4
Kane and Lombard Street	MD	8	0.15	681	238	5	21	37	68	166	170	73	43	24	10
Kearsarge Metallurgical Corp.	NH	9	0.22	7	2	8	29	46	76	174	3	2	1	1	1
Keefe Environmental Services	NH	9	0.22	12	4	7	28	45	76	174	4	2	2	1	1
Kellogg-Deering Well Field	CT	9	0.22	946	331	5	21	37	68	166	161	69	40	23	10
Kimberton Site	PA	8	0.15	308	108	5	22	37	68	167	78	34	20	11	5
Landfill & Resource Recovery	RI	9	0.22	244	86	5	22	38	69	168	43	19	11	7	3
Lindane Dump	PA	6	0.15	82	29	5	22	39	70	170	22	10	6	4	2

Dilution Factor Model Results: DNAPL Sites

Source size (acres)	0.5	10	30	100	600
Source length (m)	45	201	349	636	1,559
Aquifer thickness (m)			9.1		

		Infiltration by Hyd. Region		Average GW Velocity (m/yr)		Mixing zone depth					Dilution factor				
						Site size (acres)					Site size (acres)				
Site Name	**State**	**Region**	**(m/yr)**	**Seepage**	**Darcy**	**0.5**	**10**	**30**	**100**	**600**	**0.5**	**10**	**30**	**100**	**600**
Linemaster Switch Corp.	CT	9	0.22	1,113	389	5	21	37	68	166	189	81	47	26	11
Maryland Sand, Gravel & Stone	MD	8	0.15	2	1	10	30	46	76	174	2	1	1	1	1
McKin Co.	ME	9	0.22	890	312	5	21	37	68	166	152	65	38	21	9
Metal Banks	PA	6	0.15	5	2	8	29	46	76	174	3	1	1	1	1
Mottolo Pig Famm	NH	9	0.22	131	46	5	22	38	70	170	24	10	6	4	2
MW Manufacturing	PA	7	0.20	21,027	7,359	5	21	37	67	165	3,896	1,673	966	530	217
NCR Corp. Millsboro	DE	10	0.24	223	78	5	22	38	69	169	36	16	10	6	3
Norwood PCBS	MA	9	0.22	389	136	5	22	37	68	167	68	29	17	10	5
Nyanza Chemicals	MA	9	0.22	39	14	5	24	41	74	174	9	4	3	2	1
O'Conner Company	ME	9	0.22	214	75	5	22	38	69	169	38	16	10	6	3
Old City of York Landfill	PA	8	0.15	779	273	5	21	37	68	166	194	84	49	27	12
Old Southington Landfill	CT	7	0.20	134	47	5	22	38	70	170	27	12	7	4	2
Old Springfield Landfill	VT	9	0.22	30	11	6	25	42	74	174	7	3	2	2	1
Osborne Landfill	PA	7	0.20	1,113	389	5	21	37	68	166	208	89	52	29	12
Otis Air Natl. Guard	MA	9	0.22	312	109	5	22	38	69	168	54	24	14	8	4
Ottati & Goss/Kingston Drums	NH	9	0.22	46	16	5	24	41	73	173	10	4	3	2	1
Pease Air Force Base	NH	9	0.22	11	4	7	28	45	76	174	4	2	1	1	1
Peterson/Puritan, Inc.	RI	9	0.22	56	19	5	23	40	72	173	11	5	3	2	2
Picillo Farm	RI	9	0.22	534	187	5	22	37	68	167	92	40	23	13	6
Pinette's SalvageYard	ME	9	0.22	333	117	5	22	38	68	167	58	25	15	9	4
PSC Resources	MA	9	0.22	45	16	5	24	41	73	173	9	4	3	2	1
Re-Solve, Inc.	MA	9	0.22	834	292	5	21	37	68	166	142	61	36	20	9
Recticon/Allied Steel	PA	6	0.15	73	26	5	22	39	70	171	20	9	5	3	2
Rhinehart Tire Fire	VA	6	0.15	1,346	471	5	21	37	68	165	334	144	83	46	19
Saco Tannery Waste Pits	ME	9	0.22	56	19	5	23	40	72	173	11	5	3	2	2
Saunders Supply Co.	VA	10	0.24	28	10	6	25	42	75	174	6	3	2	2	1
Savage Mun. Water Supply	NH	9	0.22	235	82	5	22	38	69	168	42	18	11	6	3
Silresim Chemical Corp.	MA	9	0.22	26	9	6	25	42	75	174	6	3	2	2	1
Somersworth San. Landfill	NH	9	0.22	139	49	5	22	38	70	170	25	11	7	4	2
South Municipal Water Supply	NH	9	0.22	90	32	5	23	39	71	171	17	8	5	3	2
Southern MD Wood Treating	MD	10	0.24	2	1	12	30	46	76	174	2	1	1	1	1
Stamina Mills, Inc.	RI	9	0.22	2,809	983	5	21	37	67	165	475	204	118	65	27
Std. Chlorine/Tybout's Corner LF	DE	10	0.24	39	14	6	24	41	74	174	8	4	2	2	1
Strasburg Landfill	PA	8	0.15	2,160	756	5	21	37	67	165	535	230	133	73	31
Sullivan's Ledge	MA	9	0.22	112	39	5	22	39	70	171	21	9	6	4	2
Sussex County Landfill #5	DE	10	0.24	198	69	5	22	38	69	169	33	14	9	5	3
Sylvester's	NH	9	0.22	490	171	5	22	37	68	167	84	36	21	12	6
Tansitor Electronics	VT	9	0.22	103	36	5	22	39	70	171	19	8	5	3	2
Tibbets Road	NH	9	0.22	28	10	6	25	42	75	174	7	3	2	2	1
US Defense General Supply	VA	8	0.15	37	13	5	23	40	72	173	11	5	3	2	2
US Dover AFB	DE	10	0.24	4	1	10	30	46	76	174	2	1	1	1	1
US Naval Air Development	PA	6	0.15	56	19	5	23	39	71	172	16	7	4	3	2
US Newport Nav. Educ.&Tm. Ctr.	RI	9	0.22	3	1	11	30	46	76	174	2	1	1	1	1
W.R.Grace & Co./Acton	MA	9	0.22	445	156	5	22	37	68	167	77	33	20	11	5

Dilution Factor Model Results: DNAPL Sites

Source size (acres)	0.5	10	30	100	600
Source length (m)	45	201	349	636	1,559
Aquifer thickness (m)			9.1		

		Infiltration by Hyd. Region		Average GW Velocity (m/yr)		Mixing zone depth					Dilution factor				
						Site size (acres)					Site size (acres)				
Site Name	**State**	**Region**	**(m/yr)**	**Seepage**	**Darcy**	**0.5**	**10**	**30**	**100**	**600**	**0.5**	**10**	**30**	**100**	**600**
Western Sand & Gravel	RI	9	0.22	48	17	5	24	40	73	173	10	4	3	2	1
Westinghouse Elevator	PA	6	0.15	562	197	5	21	37	68	166	141	61	35	20	9
Winthrop Landfill	ME	9	0.22	16	6	6	27	44	76	174	5	2	2	1	1
Woodlawn County Landfill	MD	8	0.15	557	195	5	21	37	68	166	140	60	35	20	9

Dilution Factors (DFs) for 208 Sites in the Hydrogeologic Database (HGDB) - National Average

	Source Area (acres)				
	0.5	10	30	100	600
Source Length (m)	45	201	349	636	1,559

						Calculated Mixing Zone Depth (d)					**Dilution Factor (DF)**				
Hydrogeologic Setting	**Infiltration** (m/y)	**Average K** (m/y)	**Hyd. Grad.** (m/m)	**Darcy v** (m/y)	**Aq. Thick.** (m)	Source Area (acres)					Source Area (acres)				
						0.5	10	30	100	600	0.5	10	30	100	600
1.11	0.30	63	3.00E-02	2	30	11	41	62	96	195	3	2	2	1	1
1.11	0.30	946	1.00E-02	9	305	6	28	48	87	211	5	5	5	5	5
1.3	0.03	63	8.00E-02	5	23	5	22	39	70	172	23	23	14	8	4
1.6	0.08	946	9.30E-02	88	15	5	21	37	68	166	124	89	51	29	12
1.6	0.08	5,676	2.00E-03	11	21	5	23	39	71	173	18	17	10	6	3
1.7	0.14	157,680	1.00E-04	16	3	5	23	39	70	168	9	3	2	2	1
1.7	0.14	192,370	1.00E-02	1,924	6	5	21	37	67	165	1,459	419	242	133	55
1.8	0.03	63,072	5.00E-03	315	2	5	21	37	67	165	421	95	55	31	13
1.9	0.08	125,829	1.00E-03	126	5	5	21	37	68	166	169	39	23	13	6
1.9	0.08	2,759,400	3.00E-02	82,782	23	5	21	37	67	165	114,973	114,973	71,160	39,049	15,931
2.12	0.03	126	2.00E-03	0.3	5	8	26	42	72	170	2	1	1	1	1
2.12	0.03	946	2.00E-03	2	3	5	23	39	70	168	6	2	2	1	1
2.12	0.03	1,388	3.00E-03	4	91	5	22	39	71	174	19	19	19	19	11
2.12	0.03	1,577	1.00E-03	2	914	5	25	43	77	190	9	9	9	9	9
2.12	0.03	1,577	5.00E-03	8	24	5	22	38	69	170	35	35	23	13	6
2.12	0.03	23,652	3.00E-03	71	6	5	21	37	68	166	298	86	50	28	12
2.12	0.03	31,536	1.00E-03	32	24	5	21	37	68	166	133	133	88	49	20
2.13	0.03	95	3.00E-04	0.03	9	14	30	46	76	174	1	1	1	1	1
2.13	0.03	158	1.00E-03	0.2	130	12	50	83	138	276	3	3	2	2	2
2.13	0.03	2,838	2.00E-03	6	30	5	22	38	70	171	26	26	21	12	5
2.3	0.22	315	5.70E-03	2	46	10	40	64	104	210	3	3	2	2	1
2.3	0.22	5,992	1.00E-03	6	183	6	28	49	89	213	5	5	5	5	4
2.4	0.22	315	1.00E-03	0.3	15	18	37	52	83	180	1	1	1	1	1
2.4	0.22	315	2.00E-03	1	3	8	24	40	70	168	1	1	1	1	1
2.4	0.22	631	1.00E-02	6	9	6	26	44	76	174	5	2	2	1	1
2.4	0.22	1,892	1.00E-03	2	37	10	38	61	99	201	3	3	2	2	1
2.4	0.22	4,100	1.00E-03	4	3	6	24	40	70	168	2	1	1	1	1
2.4	0.22	11,038	2.00E-03	22	13	5	23	40	72	174	13	8	5	3	2
2.4	0.22	16,714	4.00E-03	67	6	5	22	38	69	168	35	11	7	4	2
2.4	0.22	107,222	5.00E-03	536	7	5	21	37	68	166	265	91	53	30	13

Dilution Factors (DFs) for 208 Sites in the Hydrogeologic Database (HGDB) - National Average

	Source Area (acres)				
	0.5	10	30	100	600
Source Length (m)	45	201	349	636	1,559

						Calculated Mixing Zone Depth (d)					**Dilution Factor (DF)**				
						Source Area (acres)					Source Area (acres)				
Hydrogeologic Setting	**Infiltration** (m/y)	**Average K** (m/y)	**Hyd. Grad.** (m/m)	**Darcy v** (m/y)	**Aq. Thick.** (m)	0.5	10	30	100	600	0.5	10	30	100	600
2.4	0.22	190,793	1.00E-03	191	8	5	21	37	68	167	96	35	20	12	5
2.4	0.22	3,311,280	5.00E-03	16,556	18	5	21	37	67	165	8,118	6,978	4,019	2,206	901
2.5	0.30	946	2.00E-03	2	8	10	29	45	76	173	2	1	1	1	1
2.5	0.30	1,261	3.00E-03	4	305	8	37	64	114	268	3	3	3	3	3
2.5	0.30	4,415	7.00E-04	3	38	9	37	60	98	202	3	3	2	2	1
2.5	0.30	6,938	3.00E-03	21	23	5	24	42	75	179	9	9	5	3	2
2.5	0.30	23,337	4.00E-03	93	37	5	22	38	69	170	34	34	33	19	8
2.5	0.30	56,134	2.00E-03	112	10	5	22	38	69	168	41	19	12	7	3
2.6	0.30	1,577	1.00E-03	2	12	11	33	49	79	177	2	1	1	1	1
2.6	0.30	13,876	2.80E-02	389	34	5	21	37	68	166	137	137	123	68	28
2.6	0.30	50,773	5.00E-03	254	9	5	22	37	68	167	90	39	23	13	6
2.9	0.03	126	2.00E-03	0.3	11	8	31	47	78	176	3	2	1	1	1
2.9	0.03	1,261	1.00E-04	0.1	18	12	38	55	86	183	2	1	1	1	1
2.9	0.03	3,469	2.00E-02	69	15	5	21	37	68	166	291	208	120	66	28
2.9	0.03	22,075	1.00E-03	22	91	5	22	37	68	167	94	94	94	94	52
2.9	0.03	220,752	1.00E-03	221	15	5	21	37	67	165	922	660	381	209	86
3.7	0.14	220,752	2.00E-03	442	9	5	21	37	68	165	336	145	84	46	20
3.7	0.14	296,438	2.00E-04	59	9	5	22	38	69	168	47	20	12	7	3
4.1	0.03	32	1.00E-01	3	21	5	23	40	72	174	15	14	9	5	3
4.2	0.03	22	2.80E-02	1	11	6	27	45	77	176	4	2	2	1	1
4.2	0.03	284	3.20E-03	1	3	6	24	40	70	168	3	2	1	1	1
4.4	0.14	946	8.00E-03	8	3	5	23	40	70	168	5	2	1	1	1
4.4	0.14	9,776	1.30E-02	127	3	5	21	37	68	166	63	15	9	5	3
5.2	0.03	242,827	2.00E-03	486	17	5	21	37	67	165	2,025	1,596	919	505	207
5.3	0.03	2,317,896	2.00E-03	4,636	12	5	21	37	67	165	19,317	11,072	6,377	3,500	1,428
5.8	0.03	631	3.00E-03	2	24	5	24	41	75	179	10	10	6	4	2
5.8	0.03	33,113	2.00E-06	0.07	34	18	51	70	101	199	2	1	1	1	1
6.11	0.22	1,577	1.00E-02	16	24	5	24	41	75	179	10	10	6	4	2
6.11	0.22	4,415	5.00E-03	22	15	5	23	40	72	175	13	9	5	3	2
6.11	0.22	4,415	1.00E-02	44	21	5	22	39	70	171	24	23	14	8	4

Dilution Factors (DFs) for 208 Sites in the Hydrogeologic Database (HGDB) - National Average

	Source Area (acres)				
	0.5	10	30	100	600
Source Length (m)	45	201	349	636	1,559

						Calculated Mixing Zone Depth (d)					**Dilution Factor (DF)**				
Hydrogeologic	**Infiltration**	**Average K**	**Hyd. Grad.**	**Darcy v**	**Aq. Thick.**	Source Area (acres)					Source Area (acres)				
Setting	(m/y)	(m/y)	(m/m)	(m/y)	(m)	0.5	10	30	100	600	0.5	10	30	100	600
6.11	0.22	81,994	3.00E-03	246	9	5	21	37	68	166	123	49	29	16	7
6.12	0.03	946	8.00E-03	8	6	5	22	38	69	169	34	10	6	4	2
6.12	0.03	3,154	6.00E-03	19	3	5	22	37	68	167	51	12	8	5	2
6.12	0.03	315	1.70E-02	5	9	5	22	38	70	170	24	11	7	4	2
6.14	0.22	1,577	4.00E-02	63	8	5	22	38	69	169	33	12	7	5	2
6.14	0.22	1,892	2.00E-03	4	6	7	26	43	73	171	3	2	1	1	1
6.14	0.22	5,676	1.00E-03	6	6	6	26	42	73	171	5	2	1	1	1
6.14	0.22	14,191	7.00E-04	10	18	6	25	43	77	180	7	5	3	2	2
6.14	0.22	33,113	1.00E-02	331	23	5	21	37	68	166	164	164	101	56	23
6.2	0.14	126	4.00E-03	1	8	11	29	45	75	173	2	1	1	1	1
6.2	0.14	3	1.00E-02	0.03	5	9	26	42	72	170	1	1	1	1	1
6.2	0.14	1,325	5.00E-03	7	21	6	25	43	77	182	7	6	4	3	2
6.2	0.14	2,208	3.30E-02	73	30	5	22	38	69	168	57	57	47	26	11
6.3	0.03	1,892	4.30E-02	81	6	5	21	37	68	165	341	98	57	32	14
6.3	0.03	31,536	1.40E-01	4,415	3	5	21	37	67	165	11,774	2,637	1,519	834	341
6.4	0.08	9,776	1.20E-02	117	30	5	21	37	68	166	165	165	135	75	31
6.5	0.14	63	4.00E-02	3	20	7	30	49	84	185	4	3	2	2	1
6.5	0.14	189	2.30E-02	4	61	6	27	47	85	199	5	5	5	4	2
6.5	0.14	315	5.00E-03	2	21	8	33	53	87	186	3	2	2	1	1
6.5	0.14	315	2.50E-02	8	19	6	25	42	76	180	8	6	4	3	2
6.5	0.14	31,536	5.00E-02	1,577	6	5	21	37	67	165	1,197	343	198	109	45
6.5	0.14	34,690	8.00E-03	278	5	5	21	37	68	166	203	46	27	15	7
6.8	0.14	2,208	2.50E-02	55	2	5	22	38	68	166	14	4	3	2	1
7.11	0.22	95	6.00E-03	0.6	4	9	25	41	71	169	1	1	1	1	1
7.11	0.22	2,523	2.00E-02	50	3	5	22	38	69	168	17	5	3	2	1
7.12	0.22	4,100	3.00E-03	12	32	6	25	43	77	183	8	8	6	4	2
7.12	0.22	12,614	4.90E-02	618	6	5	21	37	68	166	305	92	54	30	13
7.12	0.22	116,052	4.00E-03	464	76	5	21	37	68	166	230	230	230	230	106
7.13	0.14	3,154	1.30E-02	41	17	5	22	38	69	170	33	25	15	9	4
7.13	0.14	5,519	1.00E-02	55	`5	5	22	38	69	168	44	12	7	4	2

Dilution Factors (DFs) for 208 Sites in the Hydrogeologic Database (HGDB) - National Average

	Source Area (acres)				
	0.5	10	30	100	600
Source Length (m)	45	201	349	636	1,559

						Calculated Mixing Zone Depth (d)					Dilution Factor (DF)				
Hydrogeologic Setting	**Infiltration** (m/y)	**Average K** (m/y)	**Hyd. Grad.** (m/m)	**Darcy v** (m/y)	**Aq. Thick.** (m)	Source Area (acres)					Source Area (acres)				
						0.5	10	30	100	600	0.5	10	30	100	600
7.13	0.14	15,453	6.00E-03	93	8	5	22	37	68	167	72	27	16	9	4
7.14	0.30	6,307	4.90E-02	309	5	5	21	37	68	166	109	27	16	9	4
7.14	0.30	6,938	4.00E-03	28	8	5	23	40	72	172	12	5	3	2	1
7.14	0.30	11,038	2.50E-01	2,759	5	5	21	37	67	165	921	207	120	66	28
7.14	0.30	14,507	1.20E-02	174	18	5	22	38	68	168	62	53	31	17	8
7.14	0.30	17,660	2.00E-03	35	43	5	23	40	72	177	14	14	14	9	4
7.14	0.30	23,652	3.30E-02	781	18	5	21	37	68	166	273	234	135	75	31
7.15	0.30	7,253	6.00E-04	4	37	8	33	55	93	200	3	3	2	2	1
7.15	0.30	24,314	6.80E-03	165	11	5	22	38	68	168	59	30	18	10	5
7.16	0.14	221	4.00E-03	1	8	9	29	45	75	173	2	1	1	1	1
7.16	0.14	3,154	3.00E-03	9	9	5	24	41	73	173	9	4	3	2	1
7.17	0.14	19	8.00E-03	0.2	5	10	27	42	73	170	1	1	1	1	1
7.17	0.14	32	9.00E-03	0.3	3	8	24	40	70	168	1	1	1	1	1
7.17	0.14	32	3.00E-02	1	11	10	31	48	78	176	2	1	1	1	1
7.17	0.14	63	2.20E-02	1	3	7	24	40	70	168	2	1	1	1	1
7.17	0.14	126	1.50E-01	19	30	5	23	39	72	175	16	16	13	7	4
7.17	0.14	315	1.00E-03	0.3	12	15	33	49	79	177	2	1	1	1	1
7.17	0.14	315	7.00E-03	2	23	7	31	51	86	188	4	3	2	2	1
7.17	0.14	946	5.00E-02	47	14	5	22	38	69	169	38	24	14	8	4
7.17	0.14	3,154	1.00E-02	32	5	5	22	38	69	169	24	6	4	3	2
7.17	0.14	3,469	1.70E-02	59	55	5	22	38	69	169	47	47	47	37	16
7.17	0.14	21,760	4.00E-03	87	15	5	22	37	68	167	68	48	28	16	7
7.18	0.14	1,892	5.00E-03	9	1	5	22	38	68	166	2	1	1	1	1
7.3	0.14	946	5.00E-03	5	5	6	25	41	72	170	5	2	2	1	1
7.3	0.14	25,544	9.00E-04	23	4	5	22	39	70	168	14	4	3	2	1
7.4	0.22	189	1.20E-02	2	61	9	38	63	106	221	3	3	3	2	1
7.4	0.22	2,681	9.00E-03	24	2	5	23	39	70	167	7	2	2	1	1
7.4	0.22	3,784	4.00E-02	151	2	5	22	37	68	166	25	6	4	3	2
7.5	0.30	63	7.00E-03	0.4	518	35	143	230	363	618	2	2	2	2	1
7.5	0.30	11,038	5.00E-04	6	23	7	30	50	85	187	4	3	2	2	1

Dilution Factors (DFs) for 208 Sites in the Hydrogeologic Database (HGDB) - National Average

	Source Area (acres)				
	0.5	10	30	100	600
Source Length (m)	45	201	349	636	1,559

Hydrogeologic Setting	**Infiltration** (m/y)	**Average K** (m/y)	**Hyd. Grad.** (m/m)	**Darcy v** (m/y)	**Aq. Thick.** (m)	**Calculated Mixing Zone Depth (d)**					**Dilution Factor (DF)**				
						Source Area (acres)					Source Area (acres)				
						0.5	10	30	100	600	0.5	10	30	100	600
7.6	0.14	63	7.00E-03	0.4	4	9	25	41	71	169	1	1	1	1	1
7.6	0.14	126	1.00E-02	1	15	9	33	51	82	180	3	2	1	1	1
7.6	0.14	6,623	2.00E-02	132	21	5	21	37	68	167	102	102	59	33	14
7.7	0.14	158	3.00E-03	0.5	5	9	26	42	72	170	1	1	1	1	1
7.7	0.14	8,830	5.00E-04	4	46	6	27	47	84	195	5	5	5	3	2
7.8	0.14	631	5.00E-03	3	8	7	27	44	75	173	4	2	1	1	1
7.9	0.22	1,892	3.00E-02	57	32	5	22	38	70	170	30	30	25	14	6
7.9	0.22	2,208	9.00E-04	2	23	9	35	55	89	188	3	2	2	1	1
7.9	0.22	3,879	4.00E-03	16	8	5	24	41	73	172	10	4	3	2	1
7.9	0.22	5,676	1.00E-03	6	6	6	26	42	73	171	5	2	1	1	1
7.9	0.22	6,307	1.00E-03	6	61	6	28	48	86	201	5	5	5	4	2
7.9	0.22	7,253	6.00E-04	4	40	7	30	51	89	199	4	4	3	2	2
7.9	0.22	7,884	3.00E-02	237	3	5	21	37	68	166	75	18	11	6	3
7.9	0.22	9,776	7.00E-04	7	15	6	26	45	78	180	5	3	2	2	1
7.9	0.22	13,245	6.00E-03	79	12	5	22	38	69	169	41	23	14	8	4
7.9	0.22	13,876	2.00E-03	28	122	5	23	40	72	177	16	16	16	16	11
7.9	0.22	14,822	1.00E-03	15	61	5	24	42	76	184	9	9	9	8	4
7.9	0.22	15,768	1.00E-03	16	24	5	24	41	75	179	10	10	6	4	2
7.9	0.22	18,922	5.00E-03	95	8	5	22	38	69	168	48	18	11	6	3
7.9	0.22	23,967	2.00E-03	48	23	5	22	38	70	171	25	25	16	9	4
7.9	0.22	29,959	4.00E-03	120	19	5	22	38	68	168	61	53	31	17	8
7.9	0.22	34,374	6.00E-03	206	26	5	21	37	68	167	103	103	73	40	17
7.9	0.22	37,843	3.00E-03	114	9	5	22	38	68	168	58	25	15	9	4
7.9	0.22	44,150	2.00E-03	88	19	5	22	38	69	168	45	39	23	13	6
7.9	0.22	99,654	7.00E-04	70	7	5	22	38	69	168	36	12	7	5	2
7.9	0.22	110,376	4.00E-03	442	21	5	21	37	68	166	218	218	126	70	29
7.9	0.22	662,256	3.00E-03	1,987	6	5	21	37	67	165	976	280	162	89	37
7.9	0.22	64,018,080	9.00E-04	57,616	76	5	21	37	67	165	28,244	28,244	28,244	28,244	13,045
8.6	0.22	2,523	1.10E-02	28	6	5	23	39	71	170	16	5	3	2	2
9.12	0.22	22	4.00E-03	0.09	14	18	35	51	81	179	1	1	1	1	1

Dilution Factors (DFs) for 208 Sites in the Hydrogeologic Database (HGDB) - National Average

	Source Area (acres)				
	0.5	10	30	100	600
Source Length (m)	45	201	349	636	1,559

						Calculated Mixing Zone Depth (d)					**Dilution Factor (DF)**				
Hydrogeologic Setting	**Infiltration** (m/y)	**Average K** (m/y)	**Hyd. Grad.** (m/m)	**Darcy v** (m/y)	**Aq. Thick.** (m)	Source Area (acres)					Source Area (acres)				
						0.5	10	30	100	600	0.5	10	30	100	600
9.12	0.22	158	1.20E-02	2	3	7	24	40	70	168	2	1	1	1	1
9.13	0.30	315	6.00E-03	2	5	8	26	42	72	170	2	1	1	1	1
9.14	0.22	126	5.00E-02	6	5	6	25	41	72	170	4	2	1	1	1
9.14	0.22	126	2.00E-02	3	8	8	28	44	75	173	3	1	1	1	1
9.14	0.22	631	1.50E-01	95	2	5	22	38	68	167	22	6	4	2	2
9.14	0.22	4,100	1.00E-02	41	6	5	22	39	70	169	22	7	4	3	2
9.15	0.30	631	1.00E-02	6	11	7	28	45	77	176	4	2	2	1	1
9.15	0.30	2,208	2.00E-02	44	4	5	22	39	70	168	13	4	3	2	1
9.15	0.30	5,046	3.00E-03	15	12	6	25	42	75	176	7	4	3	2	1
9.15	0.30	11,038	7.50E-02	828	3	5	21	37	68	166	185	42	25	14	6
9.15	0.30	19,237	8.00E-03	154	12	5	22	38	69	168	55	32	19	11	5
9.15	0.30	19,237	1.30E-02	250	11	5	22	37	68	167	89	45	26	15	7
9.15	0.30	27,752	2.00E-03	56	24	5	22	39	71	172	21	21	14	8	4
9.15	0.30	27,752	2.00E-03	56	24	5	22	39	71	172	21	21	14	8	4
9.15	0.30	33,113	4.00E-04	13	30	6	26	44	79	186	7	7	5	3	2
9.15	0.30	60,864	3.00E-03	183	30	5	22	38	68	167	65	65	53	30	13
9.7	0.08	126	3.00E-02	4	107	6	25	44	79	192	7	7	7	7	4
9.9	0.22	284	1.00E-02	3	9	8	29	46	76	174	3	2	1	1	1
9.9	0.22	315	5.10E-01	161	6	5	22	37	68	167	81	24	14	8	4
9.9	0.22	8,830	4.00E-03	35	18	5	22	39	71	172	19	16	10	6	3
10.2	0.30	25	9.50E-03	0.2	5	9	26	42	72	170	1	1	1	1	1
10.2	0.30	32	1.70E-02	0.5	7	11	28	44	74	172	1	1	1	1	1
10.2	0.30	126	3.00E-03	0.4	4	9	25	41	71	169	1	1	1	1	1
10.2	0.30	126	2.50E-02	3	12	8	31	48	79	177	3	2	1	1	1
10.2	0.30	158	6.00E-04	0.1	3	8	24	40	70	168	1	1	1	1	1
10.2	0.30	284	1.00E-02	3	8	8	28	44	75	173	3	1	1	1	1
10.2	0.30	315	4.00E-03	1	6	10	27	43	73	171	2	1	1	1	1
10.2	0.30	315	1.00E-02	3	11	8	30	47	78	176	3	2	1	1	1
10.2	0.30	631	5.00E-03	3	1	6	22	38	68	166	1	1	1	1	1
10.2	0.30	2,208	1.00E-05	0.02	8	12	29	45	75	173	1	1	1	1 -	1

Dilution Factors (DFs) for 208 Sites in the Hydrogeologic Database (HGDB) - National Average

	Source Area (acres)				
	0.5	10	30	100	600
Source Length (m)	45	201	349	636	1,559

						Calculated Mixing Zone Depth (d)					**Dilution Factor (DF)**				
Hydrogeologic Setting	**Infiltration** (m/y)	**Average K** (m/y)	**Hyd. Grad.** (m/m)	**Darcy v** (m/y)	**Aq. Thick.** (m)	Source Area (acres)					Source Area (acres)				
						0.5	10	30	100	600	0.5	10	30	100	600
10.2	0.30	2,208	1.00E-02	22	8	5	24	41	73	172	10	4	3	2	1
10.2	0.30	3,469	2.00E-03	7	3	6	24	40	70	168	3	1	1	1	1
10.2	0.30	4,415	5.00E-03	22	55	5	24	42	75	183	10	10	10	7	4
10.2	0.30	4,415	1.40E-02	62	9	5	22	39	70	170	23	10	6	4	2
10.2	0.30	19,552	3.00E-04	6	21	7	30	49	84	186	4	3	2	2	1
10.2	0.30	607,068	2.00E-03	1,214	15	5	21	37	67	165	424	303	175	96	40
10.5	0.30	315	2.00E-03	0.6	3	8	24	40	70	168	1	1	1	1	1
10.5	0.30	631	1.00E-03	0.6	0	5	22	37	68	165	1	1	1	1	1
10.5	0.30	4,415	2.00E-03	9	20	6	27	46	81	183	5	4	3	2	1
11.3	0.30	631	1.00E-02	6	6	7	26	43	73	171	4	2	1	1	1
11.3	0.30	7,569	6.00E-03	45	46	5	23	39	71	174	18	18	18	12	5
11.3	0.30	12,614	5.00E-03	63	5	5	22	38	70	169	22	6	4	2	2
11.4	0.30	32	5.00E-03	0.2	15	20	37	52	83	180	1	1	1	1	1
11.4	0.30	284	3.00E-03	0.9	30	17	49	67	98	195	2	1	1	1	1
11.4	0.30	315	5.00E-02	16	2	5	23	38	69	167	3	1	1	1	1
11.4	0.30	315	1.00E-03	0.3	24	25	46	61	92	189	2	1	1	1	1
11.4	0.30	946	2.00E-04	0.2	2	6	23	39	69	167	1	1	1	1	1
11.4	0.30	1,261	2.00E-03	3	11	9	31	47	78	176	3	1	1	1	1
11.4	0.30	1,261	1.70E-02	21	3	5	23	39	70	168	6	2	2	1	1
11.4	0.30	1,577	2.30E-02	36	5	5	23	39	70	169	13	4	3	2	1
11.4	0.30	2,523	2.00E-03	5	2	6	23	39	69	167	2	1	1	1	1
11.4	0.30	3,154	1.50E-01	473	6	5	21	37	68	166	166	48	28	16	7
11.4	0.30	8,168	3.30E-03	27	6	5	23	40	72	171	11	4	3	2	1
11.4	0.30	13,876	2.00E-03	28	61	5	23	41	74	180	12	12	12	10	5
11.4	0.30	176,602	1.90E-02	3,355	4	5	21	37	67	165	1,045	235	136	75	31
12.4	0.30	309,053	5.00E-04	155	43	5	22	38	69	168	56	56	56	35	15
13.4	0.08	5,361	1.00E-03	5	6	5	24	40	72	171	9	3	2	2	1
13.4	0.08	7,884	2.00E-02	158	3	5	21	37	68	166	141	32	19	11	5

Hydrogeologic Settings for HGDB Sites

Region	Setting	Reference Number
Western Mountain Ranges		
	Mountain Slopes Facing East	1.1
	Mountain Flanks Facing East	1.3
	Mountain Flanks Facing West	1.4
	Wide Alluvial Valleys Facing East	1.6
	Wide Alluvial Valleys Facing West	1.7
	Alluvial Mountain Valleys Facing West	1.8
	Alluvial Mountain Valleys Facing East	1.9
	Coastal Beaches	1.11
Alluvial Basins		
	Mountain Slopes	2.1
	Alternating Sedimentary Rocks	2.3
	River Alluvium With Overbank Deposits	2.4
	River Alluvium Without Overbank Deposits	2.5
	Coastal Lowlands	2.6
	Alluvial Fans	2.9
	Alluvial Basins with Internal Drainage	2.13
	Playa Lakes	2.11
	Continental Deposits	2.12
Columbia Lava Plateau		
	Lava Flows: Hydraulically Connected	3.3
	Alluvial Fans	3.5
	River Alluvium	3.7
Colorado Plateau and Wyoming Basin		
	Resistant Ridges	4.1
	Consolidated Sedimentary Rocks	4.2
	Alluvium and Dune Sand	4.3
	River Alluvium	4.4
High Plains		
	River Alluvium with Overbank Deposits	5.2
	River Alluvium without Overbank Deposits	5.3
	Playa Lakes	5.7
	Ogalalla	5.8
Non-Glaciated Central Region		
	Triassic Basins	6.2
	Mountain Slopes	6.3
	Mountain Flanks	6.4

Hydrogeologic Settings for HGDB Sites

Region	Setting	Reference Number
Non-Glaciated Central Region (cont.)		
	Alternating Beds of Sandstone, Limestone, or Shale Under Thin Soil	6.5
	Alternating Beds of Sandstone, Limestone, or Shale Under Deep Regolith	6.6
	Alluvial Mountain Valleys	6.8
	Braided River Deposits	6.9
	River Alluvium with Overbank Deposits	6.14
	River Alluvium without Overbank Deposits	6.11
	Unconsolidated and Semi-Consolidated Aquifers	6.12
	Solution Limestone	6.13
Glaciated Central Region		
	Till Over Solution Limestone	7.1
	Outwash Over Solution Limestone	7.2
	Till Over Bedded Sedimentary Rock	7.3
	Thin Till Over Bedded Sedimentary Rock	7.4
	Outwash Over Bedded Sedimentary Rock	7.5
	Till Over Sandstone	7.6
	Till Over Shale	7.7
	Glaciated Lake Deposits	7.8
	Outwash	7 9
	Till Over Outwash	7.18
	Moraine	7.11
	Buried Valley	7.12
	River Alluvium with Overbank Deposits	7.13
	River Alluvium without Overbank Deposits	7.14
	Beaches, Beach Ridges, and Sand Dunes	7.15
	Swamp/Marsh	7.16
	Till	7.17
Piedmont Blue Ridge Region		
	Thick Regolith	8.1
	River Alluvium	8.6
Northeast and Superior Uplands		
	Glacial Till Over Crystalline Bedrock	9.1
	Glacial Lakes/Glacial Marine Deposits	9.2
	Bedrock Uplands	9.4
	Swamp/Marsh	9.5
	Mountain Flanks	9.7
	Glacial Till Over Outwash	9.9
	Outwash	9.15
	Alluvial Mountain Valleys	9.11

Hydrogeologic Settings for HGDB Sites

Region	Setting	Reference Number
Northeast and Superior Uplands (cont.)		
	River Alluvium with Overbank Deposits	9.12
	River Alluvium without Overbank Deposits	9.13
	Till	9.14
Atlantic and Gulf Coast		
	Confined Regional Aquifers	10.1
	Unconsolidated and Semi-Consolidated Shallow Surfacial Aquifers	10.2
	River Alluvium with Overbank Deposits	10.3
	River Alluvium without Overbank Deposits	10.4
	Swamp	10.5
Southeast Coastal Plain		
	Solution Limestone and Shallow Surfacial Aquifers	1.11
	Swamp	11.2
	Beaches and Bars	11.3
	Coastal Deposits	11.4
Hawaii		
	Volcanic Uplands	12.1
	Coastal Beaches	12.4
Alaska		
	Coastal Lowland Deposits	13.2
	Glacial and Glacio-lacustrine Deposits of the Interior Uplands	13.4

APPENDIX G

Background Discussion for Soil-Plant-Human Exposure Pathway

APPENDIX G

Background Discussion for Soil-Plant-Human Exposure Pathway

Introduction

The U.S. Environmental Protection Agency (EPA) has identified the consumption of garden fruits and vegetables as a likely exposure pathway to contaminants in residential soils. To address this pathway within the guidance, the Office of Emergency and Remedial Response (OERR) evaluated methods to calculate soil screening levels (SSLs) for the soil-plant-human exposure pathway. In particular, OERR evaluated algorithms and approaches proposed by other EPA offices or identified in the open literature. Key sources of information included the *Technical Support Document for Land Application of Sewage Sludge* (U.S. EPA, 1992), *Estimating Exposure to Dioxin-like Compounds* (U.S. EPA, 1994), *Plant Contamination* (Trapp and McFarlane, 1995), *Current Studies on Human Exposure to Chemicals with Emphasis on the Plant Route* (Paterson and Mackay, 1991), *Uptake of Organic Contaminants by Plants* (McFarlane, 1991), and *Air-to-Leaf Transfer of Organic Vapors to Plants* (Bacci and Calamari, 1991).

Although empirical data on plant uptake from soil (either through root or leaf transfer) are limited, a comprehensive collection of available empirical data on plant uptake is presented in the *Technical Support Document for the Land Application of Sewage Sludge* (U.S. EPA, 1992), hereafter referred to as the "Sludge Rule." The Sludge Rule presents uptake-response slopes, or bioconcentration factors, for a number of heavy metals found in sewage sludge, including six metals addressed in the *Soil Screening Guidance* (i.e., arsenic, cadmium, mercury, nickel, selenium, and zinc). These empirical bioconcentration factors were used in the development of the generic plant SSLs presented in this appendix.

The Sludge Rule does not present uptake-response slopes for organic chemicals because of a lack of empirical data. Therefore, generic plant SSLs for organic contaminants are not presented in this appendix. Currently, EPA is evaluating mathematical constructs to estimate plant uptake of organic chemicals for several initiatives (e.g., Hazardous Waste Identification Rule, Office of Solid Waste; Indirect Exposure to Combustion Emissions, Office of Research and Development). In addition, new mathematical models are becoming available that use a fugacity-based approach to estimate plant uptake of organic compounds (e.g., PLANTX, Trapp and McFarlane, 1995). Once these methods are reviewed and finalized, OERR may be able to address the soil-plant-human exposure pathway for organic contaminants.

The methods and data used to calculate the generic plant SSLs for arsenic, cadmium, mercury, nickel, selenium, and zinc are presented below. For comparative purposes, data on the potential phytotoxicity of metals have also been included. In addition, the site-specific factors that influence the bioavailability and uptake of metals by plants are discussed. The potentially significant effect of these site-specific factors on plant uptake underscores the need for site-specific assessments where the soil-plant-human pathway may be of concern.

G.1 SSL Calculations from Empirical Data

For uptake of chemicals into edible plants, EPA recommends a simple equation to determine SSLs for the soil-plant-human exposure pathway. The equation is appropriate for both belowground and aboveground vegetation, provided that the appropriate bioconcentration factor (Br) is used (see Section G.4). The screening level equation for the soil-plant-human pathway is given by:

SSL equation for the Soil-Plant-Human Pathway

$$\text{Screening Level (mg / kg)} = \frac{C_{\text{plant}}}{\text{Br}} \qquad \textbf{(G-1)}$$

Parameter/Definition (units)	**Default**
C_{plant}/acceptable plant concentration (mg/kg DW)	see Section G.2
Br/plant-soil bioconcentration factor (mg contaminant/kg plant tissue DW)(mg contaminant/kg soil)$^{-1}$	chemical- and plant-specific (see Section G.2)

It is important to note that the plant concentration is in dry weight (DW) instead of fresh weight (FW). Consequently, the consumption rates for plants must also be given in dry weight. For convenience, Table G-1 presents conversion factors with which to convert fresh weight to dry weight for a variety of garden fruits and vegetables. For example, because the conversion factor for lettuce is 0.052, 10 kg of lettuce fresh weight is equivalent to 0.52 kg of lettuce dry weight.

Several inputs to Equation G-1 are either derived from other equations or identified from empirical studies in the literature. Specifically, the derivation and data sources for C_{plant} and Br are discussed below.

G.2 Acceptable Concentration in Plant Tissue (C_{plant})

The acceptable contaminant concentration in plant tissues (C_{plant}) in mg/kg DW for fruits and vegetables is backcalculated using the following equation:

Acceptable Plant Concentration for Fruits and Vegetables (C_{plant})

$$C_{\text{plant}} = \frac{I \times BW}{F \times CR} \qquad \textbf{(G-2)}$$

Parameter/Definition (units)	**Default**
I/acceptable daily intake of contaminant (mg/kg-d)	see Section G.3
BW/body weight (kg)	70
F/fraction of fruits and vegetables consumed that are contaminated (unitless)	0.4 (see Section G.4)
CR/consumption rate for fruits and vegetables (kg-plant DW-d)	0.0197 (aboveground) 0.0024 (belowground) (see Section G.4)

Table G-1. Fresh-to-Dry Conversion Factors for Fruits and Aboveground Vegetables

Vegetables		Fruits	
Asparagus	0.070	Apple	0.159
Snap beans	0.111	Bushberry	0.151
Cucumber	0.039	Cherry	0.170
Eggplant	0.073	Grape	0.181
Sweet pepper	0.074	Peach	0.131
Squash	0.082	Pear	0.173
Tomato	0.059	Strawberry	0.101
Broccoli	0.101	Plum/prune	0.540
Brussels sprouts	0.151		
Cabbage	0.076		
Cauliflower	0.083		
Celery	0.063		
Escarole	0.134		
Green onions	0.124		
Lettuce	0.052		
Spinach green	0.073		
Average for vegetables	0.085	Average for fruits[a]	0.15

[a] Plum/prune was omitted from the average as an outlier.

Source: Baes et al. (1984).

G.3 Acceptable Daily Intake (I) of Contaminants

For carcinogens, the acceptable daily intake (I) in mg/kg-day is calculated at the target risk level, using default assumptions for exposure duration, exposure frequency, and averaging time. At the target risk level, the acceptable daily intake of carcinogens may be calculated as follows:

Acceptable daily intake for carcinogens

$$I = \frac{TR \times AT \times 365\, d/yr}{ED \times EF \times CSF_{oral}} \tag{G-3}$$

Parameter/Definition (units)	Default
TR/target risk level (unitless)	10^{-6}
AT/averaging time (years)	70
ED/exposure duration (years)	30
EF/exposure frequency (d/yr)	350
CSF_{oral}/oral cancer slope factor $(mg/kg\text{-}d)^{-1}$	chemical-specific (see Part 2, Table 1)

For noncarcinogens, the acceptable daily intake (I) in mg/kg-day is calculated at a hazard quotient of 1 using the following equation:

Acceptable daily intake (I) for noncarcinogens

$$I = \frac{HQ \times RfD \times AT \times 365\,d/yr}{ED \times EF} \tag{G-4}$$

Parameter/Definition (units)	**Default**
HQ/target hazard quotient (unitless)	1
AT/averaging time (years)	30
ED/exposure duration (years)	30
EF/exposure frequency (d/yr)	350
RfD/oral reference dose (mg/kg-d)	chemical-specific (see Part 2, Table 1)

G.4 Contaminated Fraction (F) and Consumption Rate (CR)

Default values for the fraction of vegetables assumed to be contaminated (F) are recommended in the *Exposure Factors Handbook* (U.S. EPA, 1990). For home gardeners, a high-end dietary fraction of 0.40 is assumed for the ingestion of contaminated fruits and vegetables grown onsite.

The default values for total fruit and vegetable consumption rates (CR) cited in the *Exposure Factors Handbook* are 0.140 and 0.2 kg/d fresh weight, respectively. Assuming that the homegrown fraction is roughly 0.25 to 0.40, EPA estimated fresh weight consumption rates of: (1) 0.088 kg/d of aboveground unprotected fruits, (2) 0.076 kg/d of aboveground unprotected vegetables, and (3) 0.028 kg/d of unprotected belowground vegetables (U.S. EPA, 1994). The consumption rates for fruits and vegetables are converted to dry weight based on the average fresh-to-dry conversion of 0.15 for fruits and 0.085 for vegetables presented in Table G-1. For unprotected belowground vegetables, the consumption rate (CR) is calculated by multiplying the fresh weight consumption rate (0.028 kg FW/d) by the average conversion factor of 0.085 resulting in a CR of 0.0024 kg DW/d. Using this same method, dry weight consumption rates of 0.0132 and 0.0065 kg DW/d were calculated for unprotected aboveground fruits and vegetables, respectively. Consequently, the overall consumption rate (CR) for aboveground, unprotected fruits and vegetables is 0.0197 kg DW/d.

The distinction between protected and unprotected produce reflects evidence that, for protected plants such as cantaloupe and citrus, there is very little translocation of contaminants to the edible parts of the plant. EPA recognizes that, while these assumptions for contaminated fraction and consumption rates are reasonable for general assessment purposes, there is likely to be wide variability on the types of produce grown at home, the percentage that is unprotected, and other exposure-related characteristics (U.S. EPA, 1994).

G.5 Soil-to-Plant Bioconcentration Factors (Br)

For metals, soil-to-plant bioconcentration factors (Br) for both aboveground and belowground plants must be identified from empirical studies because the relationship between soil concentration and plant concentration has not been described adequately to provide a mathematical construct for modeling. Table G-2 provides empirical plant uptake values for six metals identified in the *Technical Support Document for Land Application of Sewage Sludge* (U.S. EPA, 1992). Because of the variability in site-specific assessments, bioconcentration factors that are appropriate for the type of produce considered in a particular risk assessment should be selected. For general screening purposes, the geometric mean Br values for leafy vegetables and root vegetables are typically selected to represent aboveground and belowground plants, respectively. These values may be used to calculate SSLs for six metals for the soil-plant-human exposure pathway.

G.6 Example Calculation of Soil-Plant-Human SSL: Cadmium

To demonstrate how the methods described in this appendix may be used to calculate an SSL for the soil-plant-human pathway, a sample calculation is provide below for cadmium. Cadmium is considered a noncarcinogen via oral exposure and, therefore, the acceptable daily intake (I) is calculated using Equation G-4. Using the RfD for cadmium ingested in food of 1.0 x 10^{-3} mg/kg (the RfD is 5.0 x 10^{-4} in water), Equation G-4 may be solved for acceptable daily intake (I) of cadmium from a dietary source:

$$I = \frac{HQ \times RfD \times AT \times 365\ d/yr}{ED \times EF}$$

$$I = \frac{1 \times 1.0 \times 10^{-3}\ mg/kg-d \times 30\ yr \times 365\ d/yr}{30\ yrs \times 350\ d/yr}$$

$$I = 1.0 \times 10^{-3}\ mg/kg-d$$

The acceptable daily intake (I) is used in Equation G-2 to estimate the acceptable contaminant concentration in plant tissue (C_{plant}). However, Equation G-2 is designed to solve for the acceptable plant concentration (C_{plant}) in *either* aboveground fruits and vegetables or belowground vegetables. Consequently, Equations G-1 and G-2 must be combined to calculate the screening level for the ingestion of both aboveground and belowground produce. These equations are combined by summing the product of the category-specific produce intake and bioconcentration factors. Since the default contaminated fraction applies to both categories of produce, Equations G-1 and G-2 are combined to solve for the soil screening level:

(G-5)

$$\text{Screening Level}\ (mg/kg) = \frac{I \times BW}{F \times \sum(CR \times Br)}$$

Table G-2. Summary Table of Empirical Bioconcentration Factors for Metals (in mg contaminant per kg plant DW / mg contaminant per kg soil)

			Bioconcentration factors (Br)		
	Study observations	pH Range	Min	Max	Geometric Mean Br
Arsenic					
grains and cereals	1	7.5	0.026	0.026	0.026
potatoes	8	5.5 - 7.5	0.002	0.24	0.004
leafy vegetables	7	5.5 - 7.5	0.002	0.068	0.036
legumes	7	NR - 7.5	0.002	0.004	0.002
root vegetables	7	NR - 7.5	0.002	0.28	0.008
garden fruits	5	NR - 7.5	0.002	0.006	0.002
sweet corn	3	NR	0.002	0.002	0.002
Cadmium					
grains and cereals	14	4.4 - 8.0	0.002	0.346	0.36
potatoes	14	4.7- 8.0	0.002	0.076	0.008
leafy vegetables	71	4.6 - 8.4	0.002	14.12	0.364
legumes	14	5.1 - 7.7	0.002	0.054	0.004
root vegetables	25	4.6- 8.0	0.002	1.188	0.064
garden fruits	19	4.6 - 7.1	0.002	1.272	0.09
sweet corn	12	5.1 - 7.1	0.02	0.666	0.118
Mercury					
grains and cereals	1	5.3 - 7.1	0.0854	0.0854	0.0854
potatoes	1	5.3 - 7.1	0.002	0.002	0.002
leafy vegetables	9	5.3 - 7.1	0.002	0.092	0.008
legumes	3	5.3 - 7.1	0.002	0.002	0.002
root vegetables	6	5.3 - 7.1	0.002	0.086	0.014
garden fruits	7	5.3 - 7.1	0.002	0.086	0.01
sweet corn	default	ND	0.002	0.002	0.002
Nickel					
grains and cereals	10	6.2 - 8.0	0.002	0.11	0.01
potatoes	14	6.4 - 8.0	0.002	0.06	0.01
leafy vegetables	56	5.3 - 8.0	0.002	30	0.032
legumes	11	5.9 - 7.7	0.002	1.004	0.062
root vegetables	25	5.9 - 8.0	0.002	0.232	0.008
garden fruits	14	5.9 - 7.3	0.002	0.19	0.006
sweet corn	4	5.9 - 7.1	0.002	0.002	0.002
Selenium					
grains and cereals	4	5.5 - 7.0	0.002	0.11	0.002
potatoes	2	5.5 - 6.8	0.018	0.096	0.042
leafy vegetables	7	5.5 - 7.8	0.002	0.076	0.016
legumes	4	5.5 - 6.8	0.024	0.11	0.024
root vegetables	8	5.5 - 7.6	0.004	0.096	0.022
garden fruits	8	5.5 - 6.8	0.008	0.078	0.02
sweet corn	default	ND	0.002	0.002	0.002

Table G-2. (continued)

	Study observations	pH Range	Bioconcentration factors (Br)		Geometric Mean Br
			Min	Max	
Zinc					
grains and cereals	13	5.3 - 8.0	0.016	0.368	0.1
potatoes	14	4.7 - 8.0	0.01	0.122	0.024
leafy vegetables	47	4.6 - 8.0	0.012	4.488	0.25
legumes	10	5.1 - 7.7	0.002	0.11	0.036
root vegetables	20	4.6 - 8.0	0.002	0.412	0.044
garden fruits	21	4.6 - 7.3	0.002	0.394	0.046
sweet corn	8	5.1 - 6.5	0.002	0.19	0.02

NR = Not reported
ND = No data

The input parameters in Equation G-5 correspond to input parameters in Equations G-1 and G-2, with a contaminated fraction (F) of 0.4, and consumption rates (CR_{ag} and CR_{bg}) and bioconcentration factors (Br_{ag} and Br_{bg}) specific to either aboveground or belowground produce. Solving Equation G-5 for cadmium using the default parameters in Equation G-2 for F, CR_{ag}, and CR_{bg} results in:

$$\text{Screening Level} = \frac{I \times BW}{0.4 \times \Sigma(CR_{ag} \times Br_{ag}) + (CR_{bg} \times Br_{bg})}$$

$$\text{Screening Level} = \frac{1.0 \times 10^{-3}\ \text{mg/kg} - \text{d} \times 70\ \text{kg}}{0.4 \times \Sigma(0.0197 \times 0.364) + (0.0024 \times 0.064)\ \text{kg soil/d}}$$

$$\text{Screening Level} = 24\ \text{mg/kg soil}$$

As described above, the geometric mean Br values for leafy vegetables and root vegetables were selected to represent the bioconcentration factors (Br) for aboveground fruits and vegetables (Br_{ag}) and belowground vegetables (Br_{bg}), respectively (see Table G-2). SSLs for the plant pathway that are calculated using the bioconcentration factors for leafy and root vegetables are considered to be generic SSLs by OERR. During site-specific assessments, OERR recommends that a weighted average bioconcentration factor be used to reflect the type of produce grown and eaten locally.

G.7 Generic SSLs for Selected Metals

Table G-3 presents the generic SSLs for the soil-plant-human exposure pathway along with the SSLs for direct soil ingestion. In addition, this table presents plant toxicity values identified in the *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Terrestrial Plants: 1994 Revision* (Will and Suter, 1994). The phytotoxicity values are either: (1) the estimated 90th percentile of lowest observed effects concentrations (LOECs) from a data set consisting of 10 or more values, or (2) the lowest LOEC from a data set with less than 10 values. The toxicological endpoints for the phytotoxicity were limited to growth and yield parameters because they are the most common endpoints reported in phytotoxicity studies and are ecologically significant in terms of plant populations.

Table G-3. Comparison of Generic SSLs for Plant Pathway with the SSLs for Soil Ingestion and LOEC Values for Phytotoxicity (all values in mg/kg)

	Arsenic	Cadmium	Mercury	Nickel	Selenium	Zinc
Generic plant SSL	0.4	24	270	5400	2400	10000
Soil ingestion SSL	0.4	78	23	1600	390	23000
Migration to ground water SSL[a]	29(1)	8(0.4)	2(0.1)	130(7)	5(0.3)	12000(620)
Phytotoxicity LOEC	10	3	0.3	30	1	50

[a] Values based on DAF of 20 (DAF of 1).

The comparison of the generic SSLs for the plant pathway with SSLs for soil ingestion and migration to ground water suggests that this pathway may be of concern at sites contaminated with arsenic or cadmium. For mercury, nickel, and selenium, the generic plant SSLs are well above the SSLs based on soil ingestion and migration to ground water. Thus, although SSLs based on these other pathways are likely to be protective of the soil-plant-human pathway, other data suggest that phytotoxicity is likely to be the factor limiting exposure through plant uptake for these metals.

Phytotoxicity - The data in Table G-3 suggest that, for cadmium, mercury, nickel, and selenium, toxicity to plants will be observed at levels well below those estimated to elicit adverse effects in humans. The phytotoxicity of arsenic, nickel, and zinc have been well documented. However, despite the low phytotoxicity value for selenium, some authors have demonstrated that selenium can accumulate in certain plants at high levels (Bitton et al., 1980). Moreover, many phytotoxicity values are based on a reduction in yield that may result in higher levels in the surviving produce. Thus, with the exception of zinc, phytotoxicity should not be used to rule out this exposure pathway unless empirical data are available that are relevant to the site conditions (e.g., similar pH, organic matter) and the type of crops likely to be grown.

Soil Characteristics - Because the majority of the plant uptake data for metals were generated in sludge application studies, the empirical bioconcentration factors listed in Table G-2 may not be appropriate for use at all sites. For example, the adsorption "power" of sludge in the presence of phosphates, manganese, hydrous oxides of iron, and Ca^{+2} may reduce the amount of metal that is bioavailable to plants. In addition, soil pH strongly influences the ability of plants to absorb metals from soil. Several studies document that, as pH decreases, the bioavailability of many metals increases. In fact, agricultural practices maintain a soil pH of 5.5 or greater to protect against aluminum and manganese phytotoxicity. However, 40 percent of the data evaluated for the Sludge Rule were from studies in which the pH was less than 6, and, as a result, bioconcentration factors may be artificially skewed.

Chemical Characteristics - Another factor that heavily influences plant uptake of metals is the chemical form of the metal. Researchers have observed that plant uptake rates of metal salts in sludge tend to be higher than plant uptake rates in studies on elemental metals. Metal salts do not adsorb to sludge the same way as "metals in nonsalt forms" and, consequently, they are more bioavailable to plants.

Type of produce - The bioconcentration potential of metals varies with plant type. As shown in Table G-2, the range of bioconcentration factors covers an order of magnitude for most metals across the seven categories of produce. Certain types of plants are resistant to some metals while these same metals may be highly toxic to other plant species. Depending on the type of crops grown, the generic soil-plant-human SSLs may not reflect the most appropriate measures of bioconcentration.

Dietary habits - The dietary habits of the home gardener may result in an increase or decrease in exposure. The default values for consumption rate (CR) and contaminated fraction (F) represent reasonably conservative estimates for these exposure parameters. However, individual consumers may ingest significantly different quantities of produce and, depending on their fruit/vegetable preferences, may rely on crops that are efficient accumulators of metals.

G.8 SSL Calculations for Organics Lacking Empirical Data

The lack of plant bioconcentration data on organics presented in the *Technical Support Document for Land Application of Sewage Sludge* (U.S. EPA, 1992) has been discussed in several other sources. For example, the status of empirical data on plant uptake and accumulation of organics was recently evaluated for a database on uptake/accumulation, translocation, adhesion, and biotransformation of chemicals in plants (Nellessen and Fletcher, 1993). This database, referred to as UTAB, is one of the most comprehensive data sources available on chemical processes in plants and contains over 42,000 records taken from more than 2,100 published papers. The authors found that, with the exception of pesticides, uptake-response data for organic chemicals are available for roughly 25 percent of the chemicals monitored by EPA. Given the comprehensive nature of the UTAB database, modeling may be the only alternative to evaluating the soil-plant-human pathway in the near future for many organic chemicals.

Recently, several authors have developed models to predict the uptake and accumulation of organic chemicals in plants (e.g., Matthies and Behrendt, 1994; McKone, 1994; Trapp et al., 1994). One of the most promising models for use as a risk assessment tool is PLANTX, a peer-reviewed partitioning model that describes the dynamic uptake from soil, or solution, and the metabolism and accumulation of xenobiotic chemicals in roots, stems, leaves, and fruits (Trapp et al., 1994). Unlike a number of other models used to estimate plant uptake, PLANTX is not based on regression equations that correlate log K_{ow} with plant bioconcentration; it is a mechanistic model that accounts for major plant processes and requires only a few well-known input data. Moreover, it was designed as a risk assessment tool and has been validated for the herbicide bromicil and several nitrobenzenes. A follow-on model (PLANTE) has recently been made available that also incorporates plant uptake during transpiration (i.e., accumulation directly from the air). The results on bromocil, nitrobenzene, etc., as well as ongoing validation studies suggest that the PLANT models may be a scientifically defensible alternative to the uptake-response slopes generated by log K_{ow} regressions.

G.9 Conclusions and Recommendations

The comparison of generic plant SSLs with generic SSLs for soil ingestion and migration to ground water indicate that the soil-plant-human exposure pathway may be of concern for two of the six metals evaluated (arsenic and cadmium). For mercury, nickel, and selenium, SSLs based on the other pathways are likely to be adequately protective of the soil-plant-human exposure pathway. In addition, data presented on the phytotoxicity of these metals and zinc suggest that toxic effects in plants are likely to be observed below levels that would be harmful to humans. Although this pathway may not be of concern from a human health standpoint, these data suggest that metals could be of particular concern for ecological receptors.

Currently, EPA is developing methods to evaluate the uptake of organics into plants. In addition to the efforts of the Office of Solid Waste and the Office of Research and Development mentioned in the Introduction, OERR has jointly funded research on plant uptake of organics with the State of California. These studies support ongoing revisions to the indirect, multimedia exposure model, CalTOX. Until these efforts are reviewed and finalized, OERR will continue to address the potential for plant uptake of organics on a case-by-case basis.

References

Bacci, Eros, and David Calamari. 1991. Air-to-leaf transfer of organic vapors to plants. In: *Municipal Waste Incineration Risk Assessment.* C.C. Travis editor, Plenum Press, New York.

Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. *Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides Through Agriculture*. Oak Ridge National Laboratory, Oak Ridge, TN.

Bitton, G., B.L. Damron, G.T. Edds, and J.M. Davidson. 1980. *Sludge -- Health Risks of Land Application*. Ann Arbor Science Publishers, Inc., Ann Arbor, MI.

Matthies, M., and H. Behrendt. 1994. Dynamics of leaching, uptake, and translocation: The Simulation Model Network Atmosphere-plant-soil (SNAPS). In: *Plant Contamination: Modeling and Simulation of Organic Chemical Processes*. Stefan Trapp and J. Craig Mc Farlane eds, Lewis Publishers, Michigan.

McKone, T. 1994. Uncertainty and variability in human exposures to soil contaminants through homegrown food: a Monte carlo assessment. *Risk Analysis* 14 (4): 449-463.

McFarlane, Craig. 1991. Uptake of organic contaminants by plants. In: *Municipal Waste Incineration Risk Assessment*. C.C. Travis editor, Plenum Press, New York.

Nellessen, J.E., and J.S. Fletcher. 1993. Assessment of published literature pertaining to the uptake/accumulation, translocation, adhesion and biotransformation of organic chemicals by vascular plants. *Environmental Toxicology and Chemistry* 12: 2045-2052.

Paterson, Sally and Donald Mackay. 1991. Current studies on human exposure to chemicals with emphasis on the plant route. In: *Municipal Waste Incineration Risk Assessment.* C.C. Travis editor, Plenum Press, New York.

Trapp, S., and J.C. McFarlane. 1995. *Plant Contamination. Modeling and Simulation of Organic Chemical Processes.* Lewis Publishers, Boca Raton, FL.

Trapp, S., and J.C. McFarlane, and M. Matthies. 1994. Model for uptake of xenobiotic into plants: Validation with bromocil experiments. *Environmental Toxicology and Chemistry* 13 (3): 413-422.

Travis, C.C., and A.D. Arms. 1988. Bioconcentration of organics in beef, milk and vegetation. *Environmental Science and Technology* 22(3):271-274.

U.S. EPA (Environmental Protection Agency). 1990. *Exposure Factors Handbook*. Office of Health and Environmental Assessment, Exposure Assessment Group, Washington, DC. March.

U.S. EPA (Environmental Protection Agency). 1992. *Technical Support Document for Land Application of Sewage Sludge, Volume I and II*. EPA 822/R-93-001a. Office of Water, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1994. *Estimating Exposure to Dioxin-like Compounds. Volumes I-III: Site-specific Assessment Procedures*. EPA/600/6-88/005C. Office of Research and Development, Washington, DC. June.

Will, M.E. and G.W. Suter II. 1994. *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Terrestrial Plants: 1994 Revision*. ES/ER/TM-85/R1. Prepared for the U.S. Department of Energy by the Environmental Sciences Division of the Oak Ridge National Laboratory.

APPENDIX H

Evaluation of the Effect on the Draft SSLs of the Johnson and Ettinger Model (EQ, 1994a)

ENVIRONMENTAL QUALITY MANAGEMENT, INC.

MEMORANDUM

TO: Janine Dinan

DATE: October 7, 1994

SUBJECT: Evaluation of the Effect on the Draft SSLs of the Johnson and Ettinger (1991) Model for the Intrusion of Contaminant Vapors Into Buildings

FROM: Craig S. Mann

FILE: 5099-3

cc:

Under U.S. Environmental Protection Agency (EPA) Contract No. 68-D3-0035, Task order No. 0-25, Environmental Quality Management, Inc. (EQ) was directed to evaluate the effect on the draft soil screening levels (SSLs) of employing the Johnson and Ettinger (1991) model for estimating the intrusion rate of contaminant vapors from soil into buildings. This memorandum summarizes the evaluation.

Model Review:

Johnson and Ettinger (1991) is a closed-form analytical solution for both convective and diffusive transport of vapor-phase contaminants fully incorporated in soil into enclosed structures. The nondimensionalized mass balance is written as:

$$\frac{\partial \sum_{i} \in_i C_i^*}{\partial t^*} - \left(\frac{L_p}{L_D}\right)\left(\nabla^* P^*\right) \cdot \left(\nabla^* C_v^*\right) = \nabla^* \cdot \left[\frac{D^{eff}\,\mu\, L_p}{k_v\, \Delta P_r\, L_D}\right] \nabla^* C_v^* + \sum_{i} R_i^* \qquad (1)$$

where $*$ = Nondimensional variables

$\in_i$ = Volume fraction of phase i, unitless

C_i = Concentration of contaminant in phase i, g/cm^3

t = Time, s

L_P = Convection path length, cm

L_D = Diffusion path length, cm

P = Pressure in vapor-phase, g/cm-s^2

∇ = Del operator, 1/cm

C_v = Contaminant concentration in vapor phase, g/cm3

D^{eff} = Effective diffusion coefficient, cm^2/s

μ = Vapor viscosity, g/cm-s

k_v = Soil permeability to vapor flow, cm^2

ΔP_r = Reference indoor-outdoor pressure differential, $g/cm\text{-}s^2$

R_i = Formation rate of contaminant in phase i, $g/cm^3\text{-}s$

and,

C_i^* = C_i/C_r

∇^* = $L_D \nabla$

P^* = $P/\Delta P_r$

t^* = $t\,(k_v \Delta P_r / L_D L_P \mu)$

R_i^* = $R_i L_D L_P \mu / C_r k_r \Delta P_r$

where C_r, L_P and L_D are characteristic concentration, convection pathway length, and diffusion pathway length, chosen to give the dependent concentration variable and derivatives of C_i^* and P^* magnitudes of order unity.

The mass balance solution includes the following assumptions:

1. The soil column is isotropic within any horizontal plane.
2. The effective diffusion coefficient is constant within any horizontal plane.
3. Concentration at the soil-air interface is zero (i.e., boundary layer resistance is zero).
4. No loss of contaminant occurs across the lower boundary (i.e., no leaching).
5. Source degradation and transformation are not considered.
6. Convective vapor flow near the building foundation is uniform.
7. Contaminant vapors enter the building primarily through openings in the walls and foundation at or below grade.
8. Convective velocities decrease with increasing contaminant source-building distance.
9. All contaminant vapors directly below a basement will enter the basement, unless the floor and walls are perfect vapor barriers.

10. The building contains no other contaminant sources or sinks, and the air volume is well mixed.

Therefore,

$$Q_{building}\, C_{building} = E \tag{2}$$

where $Q_{building}$, $C_{building}$, and E represent the volumetric flow rate or ventilation rate of the building (cm^3/s), contaminant concentration within the building (g/cm^3), and rate of contaminant entry (g/s), respectively.

Also,

$$\alpha = Q_{building}/C_{source} \tag{3}$$

where C_{source} is the vapor-phase contaminant concentration within the soil at the source, and α represents the attenuation coefficient. C_{source} is written as:

$$C_{source} = \frac{H\, C_s\, \rho_b}{\Theta_w + K_d \rho_b + H\Theta_a} \tag{4}$$

where H = Henry's law constant, unitless

C_s = Soil bulk concentration, g/g

ρ_b = Soil dry bulk density, g/cm^3

Θ_w = Soil water-filled porosity, unitless

K_d = Soil-water partion coefficient, cm^3/g

Θ_a = Soil air-filled porosity, unitless.

The authors derive a solution for α for both steady-state conditions (i.e., depth of contamination, $z = \infty$) and for quasi-steady-state conditions ($0 < z < L$). For steady-state conditions α is written as:

$$\alpha = \left[\left[\frac{D^{eff}\, A_B}{Q_{\,building}\, L_T}\right] x \exp\left(\frac{Q_{soil}\, L_{crack}}{D^{crack}\, A_{crack}}\right)\right] /$$

$$\left[\exp\left(\frac{Q_{soil}\, L_{crack}}{D^{crack}\, A_{crack}}\right) + \left[\frac{D^{eff}\, A_B}{Q_{building}\, L_T}\right] + \left[\frac{D^{eff}\, A_B}{Q_{soil}\, L_T}\right]\left[\exp\left(\frac{Q_{soil}\, L_{crack}}{D^{crack}\, A_{crack}}\right) - 1\right]\right] \tag{5}$$

where D^{eff} = Effective diffusion coefficient, cm^2/s

A_B = Area of basement, cm^2

L^T = Source-building separation, cm

Q_{soil} = Volumetric flow rate of soil gas into the building, cm^3/s

L_{Crack} = Building foundation thickness, cm

D^{Crack} = Effective diffusion coefficient through crack, cm^2/s ($D^{Crack} = D^{eff}$)

A_{Crack} = Area of crack, cm^2

$Q_{building}$ = Building ventilation rate, cm^3/s.

For quasi-steady-state conditions the long-term average attenuation coefficient <a> is:

$$<\alpha> \;=\; \frac{\rho_b\ C_R\ \Delta H_C\ A_B}{Q_{building}\ C_{source}\ \tau}\left(\frac{L_T^0}{\Delta H_C}\right)\left[\left(\beta^2\ +\ 2\Psi\tau\right)^{1/2}\ -\ \beta\right] \tag{6}$$

where ρ_b = Soil dry bulk density, g/cm^3

C_R = Average contaminant level in soil, g/g

ΔH_c = Thickness of depth over which contaminant is distributed, cm

A_B = Area of basement, cm^2

$Q_{building}$ = Building ventilation rate, cm^3/s

C_{source} = Vapor-phase soil concentration at source, g/cm^3

τ = Exposure averaging period, s

L_T^0 = Source-building separation at t=0, cm

and,

$$\beta \;=\; \left(\frac{D^{eff}\ A_B}{L_T^0\ Q_{soil}}\right)\left[1\ -\ \exp\left(-\ \frac{Q_{soil}\ L_{crack}}{D^{crack}\ A_{crack}}\right)\right]\ +\ 1 \tag{7}$$

$$\Psi \;=\; D^{eff}\ C_{source}/\left(L_T^0\right)^2\ \rho_b\ C_R \tag{8}$$

The time required to deplete a finite source (τ_D) of depth ΔH_c is given as:

$$\tau_D = \frac{[\Delta H_C / L_T^0 + \beta] - \beta^2}{2\Psi} \tag{9}$$

If the exposure period (τ) is greater than τ_D, the average emission rate into the building <E> is given as a simple mass balance:

$$<E> = \rho_b \, C_R \, \Delta H_C \, A_B \, / \, \tau \tag{10}$$

and the average building concentration ($C_{building}$) is:

$$C_{building} = <E>/Q_{building} \tag{11}$$

Evaluation

In order to evaluate the effects of using the model on the SSLs for volatile contaminants, a case example was constructed which best estimates a reasonable high end exposure point concentration for residential land use. Where possible, values of model variables were taken directly from Johnson and Ettinger (1991).

The case example assumes that a residential dwelling with a basement is constructed within the area of homogeneous residual contamination such that the contaminant source lies directly below the basement floor at t = 0. Therefore, the diffusion and convection path lengths were set equal to the thickness of the basement slab (15 cm). Soil permeability to vapor flow from the basement floor to the bottom of contamination was set equal to 1.0 x 10^{-8} cm^2 (1 darcy) which is representative of silty to fine sand. Soil column-building pressure differential was set equal to 1 pascal (10g/cm-s^2) as a reasonable long-term average value (Johnson and Ettinger, 1991). Values for all other soil properties were set equal to those of the Generic SSLs in the July 1994 Technical Background Document for Draft Soil Screening Level Framework (TBD). Building variables, i.e., basement area, ventilation rate, etc., were taken from Johnson and Ettinger (1991).

In the analysis, the values for $C_{building}$ (kg/m^3) were calculated for the 42 chemicals in the TBD for which human health benchmarks are available. Please note that the values of C_{source} and $C_{building}$ were calculated for an initial soil concentration of 1 mg/kg instead of 1 x 10^{-6} g/g. This was done to facilitate reverse calculation of the SSL in units of mg/kg. Therefore, these values are artificially high by a factor of 1 x 10^6. The inverse of the value of $C_{building}$ (m^3/kg) was used as the indoor volatilization factor (VF_{indoor}) and substituted into Equations 2-4 or 2-5 of the TBD as appropriate to calculate the resulting carcinogenic and noncarcinogenic inhalation SSLs. SSLs were calculated for both steadystate conditions (infinite source depth) and quasi-steady-state conditions (finite source depth). In each case were the exposure period exceeded the time required for source depletion (finite source depth), the volatilization factor was normalized to an average contaminant level in soil (C_r) of 1 mg/kg. For quasi-steady-state conditions, the depth to the bottom of contamination was set equal to 2 meters below the basement floor.

The value of the indoor SSL for each contaminant was compared to the respective SSL calculated for outdoor exposures of the same duration using the Generic SSL calculations found in the TBD. The outdoor SSLs were computed for a 30 acre square area source of emissions. Table 1 summarizes the results of this comparison. The attachment to this memorandum gives the detailed computations for this evaluation.

TABLE 1.
SUMMARY OF INDOOR AND OUTDOOR INHALATION SSLs FOR VOLATILE CONTAMINANTS

Chemical	Indoor SSL, infinite source (mg/kg)	Indoor SSL, finite source (mg/kg)	Outdoor SSL, infinite source (mg/kg)
Aldrin	0.4	0.4	0.5
Benzene	0.002	0.02	0.5
Bis(2-chloroethyl)ether	0.02	0.05	0.3
Bromoform	0.8	0.9	43
Carbon disulfide	0.03	0 7	11
Carbon tetrachloride	0.0007	0.01	0.2
Chlordane	51	53	54
Chlorobenzene	0.7	2	87
Chloroform	0.001	0.007	0.2
DDT	5[a]	5[a]	5[a]
1,2-Dichlorobenzene	26	65	297[a]
1,4-Dichlorobenzene	102	235[a]	235[a]
1,1-Dichloroethane	4	35	939
1,2-Dichloroethane	0.002	0.007	0.3
1,1-Dichloroethylene	0.0001	0.003	0.04
1,2-Dichloropropane	0.06	0.3	10
1,3-Dichloropropene	0.0007	0.004	0.1
Dieldrin	3	4	2
Ethylbenzene	21	69	257[a]
Heptachlor	0.04	0.04	0.3
Heptachlor epoxide	1	1	1
Hexachloro-1,3-butadiene	0.03	0.05	1
Hexachlorobenzene	0.3	0.6	1
HCH-alpha(alpha-BHC)	0.5	0.6	0.9
HCH-beta(beta-BHC)	7[a]	7[a]	7[a]
Hexachlorocyclopentadiene	0.06	0.07	2
Hexachloroethane	0.6	0.6	45
Methyl bromide	0.01	0.3	3
Methylene chloride	0.04	0.3	7
Nitrobenzene	9	25	100
Styrene	185	472	1439[a]
1,1,2,2-Tetrachloroethane	0.007	0.02	0.4
Tetrachloroethylene	0.05	0.3	11
Toluene	6	28	521[a]
Toxaphene	2	2	2[a]
1,2,4-Trichlorobenzene	6	9	214
1,1,1-Trichloroethane	5	69	980[a]
1,1,2-Trichloroethane	0.009	0.02	1
Trichloroethylene	0.01	0.09	3
2,4,6-Trichlorophenol	64	94	190
Vinyl acetate	5	14	351
Vinyl chloride	0.00002	0.002	0.01

[a] = SSL based on C_{sat}

As can be seen from Table 1, results on a chemical-specific basis indicate a rate of change as high as three orders of magnitude between the outdoor SSL and the infinite source indoor SSLs in the case of highly volatile contaminants. For very persistent contaminants, the relative difference was considerably less, and in some cases there was no difference in SSL concentrations.

This variability is due to: 1) the variability in the human health benchmarks used to calculate the risk-based SSLs, and 2) the apparent diffusion coefficient of each compound. The apparent diffusion coefficient can be expressed as the effective diffusion coefficient through soil divided by the liquid-phase partition coefficient (Jury et al., 1983). The apparent diffusion coefficient (D_A) is given here so as not to be confused with the effective diffusion coefficient (D^{eff}) from Johnson and Ettinger (1991):

$$DA = \left[\left(\Theta_a^{10/3}\ D_a\ H + \Theta_w^{10/3}\ D_w\right) / \Theta_t^2\right] / (\rho_b\ K_d + \Theta_w + \Theta_a H) \qquad (12)$$

where D_A = Apparent diffusion coefficient, cm^2/s

Θ_a = Air-filled soil porosity, unitless

D_a = Diffusivity in air, cm^2/s

H = Henry's law constant, unitless

Θ_w = Water-filled soil porosity, unitless

D_w = Diffusivity in water, cm^2/s

Θ_t = Total soil porosity, unitless

ρ_b = Soil dry bulk density, g/cm^3

K_d = Soil-water partition coefficient, cm3/g.

With all nonchemical-specific variables held constant, Figure 1 shows the exponential relationship between the apparent diffusion coefficient and the building concentration for quasi-steady-state conditions (finite source).

For nonchemical-specific variables, a sensitivity analysis was performed for soil permeability to vapor flow (k_v), soil-building pressure differential (Δ P), depth of contamination (ΔH_c), source-building separation at t = 0 (L_T^0), crack-to-total area ratio (η), and building ventilation rate ($Q_{building}$).

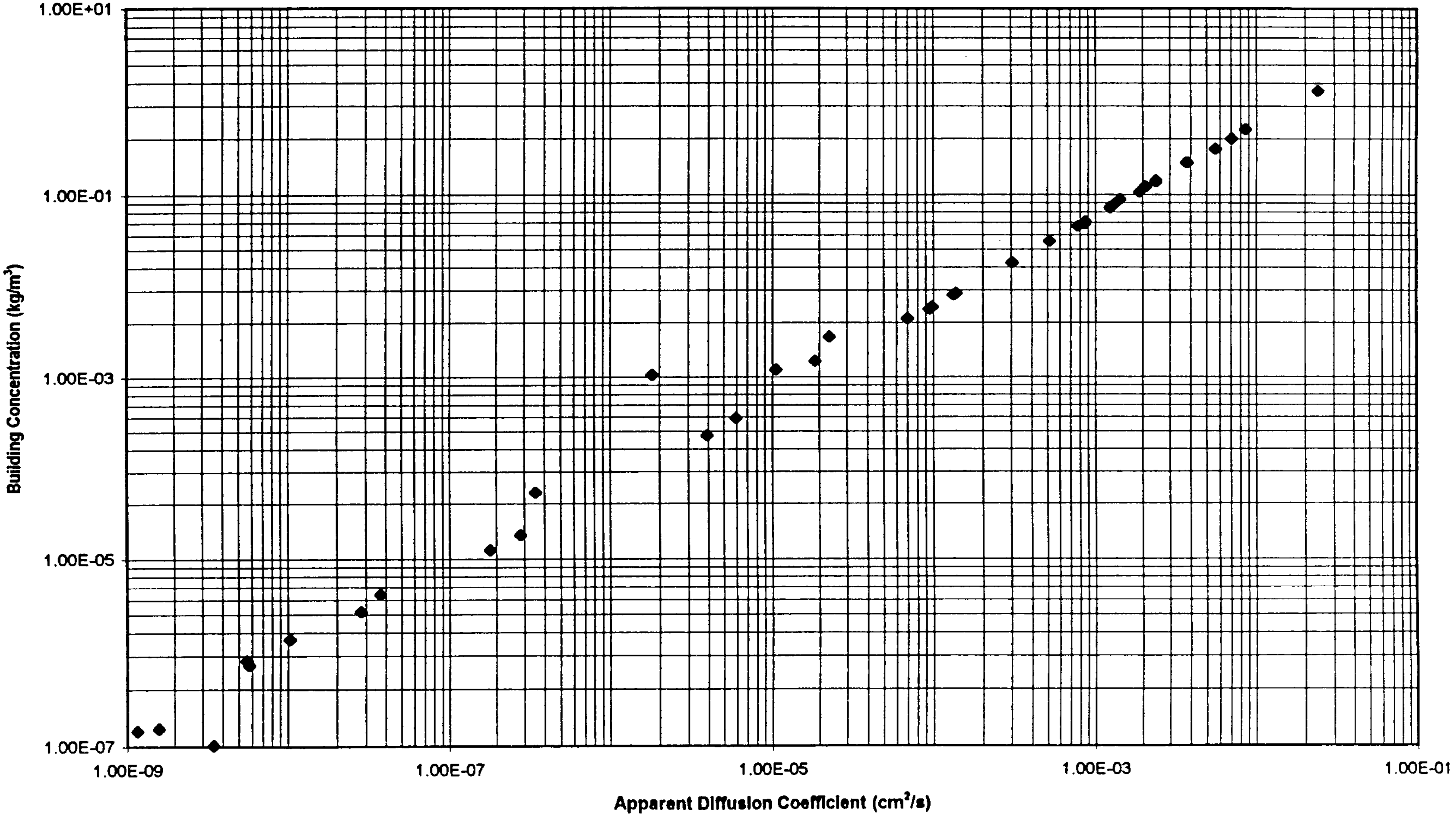


Figure 1
Building Concentration Versus Apparent Diffusion Coefficient

Table 2 shows the results of the sensitivity analysis for the quasi-steady-state condition (finite source). As can be seen from Table 2, the effect of the building ventilation rate is linear if the value of C_{sat} is not included in limiting the value of the SSL. Depth of contamination (ΔH_c) has the greatest effect for contaminants with higher apparent diffusion coefficients (e.g., benzene, chloroform, vinyl chloride, etc.), in that as ΔH_c increases, the time required for source depletion (τ_D) also increases. Therefore, with greater initial contaminant mass in the soil, these compounds are emitted for a longer period of time thus reducing the SSL. For the more persistent contaminants, an increase in k_v or ΔP produces the greatest results. This is to be expected as values of τ_D for these contaminants exceed the exposure duration. Table 2 also indicates that an order of magnitude change in values Of L_T^0 and η produce same order of magnitude results. It must be remembered, however, that in the case of L_T^0, the model assumes isotropic soil conditions from the point of building entry to the bottom of contamination. As L_T^0 increases, α decreases until diffusion not convection limits the rate of contaminant vapor transport. The effect of changes in the value of η decrease as values of k_v decrease such that for very permeable soils and convection-dominated vapor transport, the effect of crack size is relatively insignificant.

Conclusions

Use of the Johnson and Ettinger (1991) model to calculate SSLs based on indoor chronic exposures can have significant impacts on the values of the SSLs for contaminants with high apparent diffusion coefficients. When comparing the infinite source indoor model to the infinite source outdoor model for these contaminants, values of the SSL differ by orders of magnitude for case example conditions. Under these conditions, diffusion is the limiting transport mechanisms for all but one contaminant for both steady-state and quasi-steady-state conditions. To effect case example conditions, the following must be true:

1. The contaminant source must be relatively close or directly beneath the structure.
2. The soil between the structure and the source must be very permeable (k_v, $\geq 10^{-8}$ cm^2).
3. The structure must be underpressurized.
4. The air within the structure must be well mixed (i.e., little or no soil-air boundary layer resistance).
5. The combination of diffusion coefficient through the cracks, area of the cracks, and building underpressurization must offer no more resistance than the soil column beneath the structure.

From this evaluation, the four most important factors affecting the average long-term building concentration and thus the SSL are building ventilation rate, source-building separation, soil permeability to vapor flow, and source depth. If the source of contamination is relatively deep and close to the building, and if the soil between the source and the building is very permeable, building concentrations of contaminants with relatively high apparent diffusion coefficients will increase dramatically.

TABLE 2.
MODEL SENSITIVITY TO NONCHEMICAL SPECIFIC VARIABLES

			Ratio of Variable-to-Test Condition SSL					
Chemical	Apparent diffusion coefficient, D_A (cm^2/s)	Test condition SSL, (mg/kg)	Soil vapor permeability, k_v x 10	Soil-bldg. pressure differential, ΔP x 10	Depth to source lower boundary, ΔH_c x 10	Source-bldg. separation at t=0, L_T^0 x 10	Inverse of crack-to-total area ratio, $1/\eta$ x 10	Bldg. ventilation rate, $Q_{building}$ x 10
DDT	1.16E-09	5[a]	1	1	1	1	1	1.0
Dieldrin	1.59E-09	4	0.1	0.1	1	1.2	1.5	3.4
HCH-beta(beta-BHC)	3.54E-09	7[a]	0.8	0.8	1	1	1	1.0
Chlordane	5.63E-09	53	0.1	0.1	1	1.3	1.3	1.3
Heptachlor epoxide	5 78E-09	1	0.1	0.1	1	1.3	1.5	8.4
Aldrin	1.03E-08	0.4	0.1	0.1	1	1.2	1.5	10
HCH-alpha(alpha-BHC)	2.81E-08	0.6	0.1	0.1	1	1.2	1.5	10
Toxaphene	3.69E-08	2	0.1	0.1	1	1.1	1.1	1.1
2,4,6-Trichlorophenol	1.81E-07	94	0.1	0.1	1	1.1	1.5	10
Hexachlorobenzene	284E-07	0.6	0.1	0.1	1	1.1	1.5	3.2
Heptachlor	3.52E-07	0.04	0.1	0.1	1	1.3	1.5	10
Hexachloroethane	1.80E-06	0.6	0.3	0.3	1	2	1.4	10
Nitrobenzene	3.92E-06	25	0.1	0.1	1	1	1.5	10
Bis(2-chloroethyl)ether	5.94E-06	0.05	0.1	0.1	1	1	1.5	10
Hexachlorocyclo-pentadiene	1.06E-05	0.07	0.2	0.2	1	1.2	1.5	10
1,2,4-Trichlorobenzene	1.89E-05	9	0.1	0.1	1	1.1	1.5	10
Bromoform	2.32E-05	0.9	0.2	0.2	1	1.2	1.5	10
Hexachloro-1,3-butadiene	6.97E-05	0.05	0.1	0.1	1	1.1	1.5	10
Styrene	9.50E-05	472	0.1	0.1	1	1	1 5	3.0
1,1,2,2-Tetrachloroethane	9.89E-05	0.02	0.2	0 2	1	1	1 5	10
1,2-Dichlorobenzene	1.34E-04	65	0.2	0.2	1	1	1.5	4.5
1,4-Dichlorobenzene	1.38E-04	235[a]	0.2	0.2	1	1	1	1.0
1,1,2-Trichloroethane	3.04E-04	0.02	0.4	0.4	1	1	1.5	10
Chlorobenzene	5.18E-04	2	0.8	0.8	1	1	1.5	10
Vinyl acetate	7.79E-04	14	1	1	1	1	1.5	10
1,2-Dichloropropane	8.57E-04	0.007	0.9	0.9	1	1	1.5	10
Ethylbenzene	8.64E-04	69	1	1	0.8	1	1.2	3.7
1,2-Dichbropropane	1.24E-03	0.3	1	1	0.6	1	1	10
Toluene	1.25E-03	28	1	1	0.7	1	1	10
Tetrachloroethylene	1.34E-03	0.3	1	1	0.5	1	1	10
1,3-Dichloropropene	1.44E-03	0.004	1	1	0.4	1	1	10
Chloroform	1.91E-03	0.007	1	1	0.5	1	1	10
1,1-Dichloroethane	2.08E-03	35	1	1	0.4	1	1	10
Benzene	2.12E-03	0.02	1	1	0.4	1	1	10
Trichloroethylene	2.44E-03	0.09	1	1	0.3	1	1	10
Methylene chloride	2.45E-03	0.3	1	1	0.4	1	1	10
1,1,1-Trichioroethane	3.79E-03	69	1	1	0.2	1	1	10
Carbon tetrachloride	3.82E-03	0.01	1	1	0.2	1	1	10
Carbon disulfide	5.67E-03	0.7	1	1	0.2	1	1	10
1,1-Dichloroethylene	7.09E-03	0.003	1	1	0.1	1	1	10
Methyl bromide	8.56E-03	0.3	1	1	0.1	1	1	10
Vinyl chloride	2.40E-02	0.002	1	1	0.1	1	1	10

[a] = SSL based C_{sat}

It should be noted, however, that soil permeability, k_V, is the most variable parameter at any given site, and may vary by three orders of magnitude across a typical residential lot (Johnson and Ettinger, 1991). For this reason, the overall effective diffusion coefficient should be determined by integration across each soil type. Overall diffusion/convection vapor transport will therefore be limited by the soil stratum offering the greatest resistance to vapor flow.

References

Johnson, Paul C., and Robert A. Ettinger. 1991. Heuristic model for predicting the intrusion rate of contaminant vapors into buildings. Environ. Sci. Technol., 25(8):1445-1452.

Jury, W. A., W. J. Farmer, and W. F. Spencer. 1983. Behavior Assessment Model for Trace Organics in Soil, l, Model description. J. Environ. Qual., 12:558-564.

Attachment

ATTACHMENT

DETAILED MODEL EVALUATION

COMPARISON OF INDOOR AND OUTDOOR INHALATION SSLs FOR VOLATILE CONTAMINANTS

Chemical	CAS No.	Soil bulk density, ρ_b (g/cm^3)	Soil moisture, w (g/g)	Soil moisutre, Θ_w (cm^3/cm^3)	Soil total porosity, η (unitless)	Soil air-filled porosity, Θ_a (unitless)	Soil water-filled porosity, Θ_w (unitless)	Diffusivity in air, D_a (cm^2/s)	Diffusity in water, D_w (cm^2/s)	Effective diffusion coeffi-cient, D_o (cm^2/s)	Soil vapor permea-bility, K_v (cm^3)	Soil-bldg. pressure differen-tial ΔP (g/cm-s^2)	Diffusion path length, L_d (cm)	Convec-tion path length, L_p (cm)	Vapor viscosity, μ (g/cm-s)	Peclet number, Pe (unitless)	Henry's law constant, H (unitless)	Organic carbon partition coeffi-cient, K_{oc} (cm^3/g)
Aldrin	309-00-2	1.5	0.1	0.15	0.434	0.284	0.150	1.32E-02	4.86E-06	1.05E-03	1.00E-08	10	15	15	1.80E-04	0.53	4.20E-03	4.84E+04
Benzene	71-43-2	1.5	0.1	0.15	0.434	0.284	0.150	8.70E 02	9.80E-066	6.95E-03	1.00E-08	10	15	15	1.80E-04	0.08	2.20E-01	5.70E+01
Bis(2-chloroethyl)ether	111-44-4	1.5	0.1	0.15	0.434	0.284	0.150	6.92E-02	7.53E-06	5.53E-03	1.00E-08	10	15	15	1.80E-04	0.10	8.80E-04	7.60E+01
Bromoform	75-25-2	1.5	0.1	0.15	0.434	0.284	0.150	1.49E-02	1.03E-05	1.19E-03	1.00E-08	10	15	15	1.80E-04	0.47	2.50E-02	1.26E+02
Carbon disulfide	75-15-0	1.5	0.1	0.15	0.434	0.284	0.150	1.04E-01	1.00E-05	8.31E-03	1.00E-08	10	15	15	1.80E-04	0.07	5.20E-01	5.20E+01
Carbon tetrachloride	56-23-5	1.5	0.1	0.15	0.434	0.284	0.150	7.80E-02	8.80E-06	6.23E-03	1.00E-08	10	15	15	1.80E-04	0.09	1.20E+00	1.64E+02
Chlordane	57-74-9	1.5	0.1	0.15	0.434	0.284	0.150	1.18E-02	4.37E-06	9.43E-04	1.00E-08	10	15	15	1.80E-04	0.59	2.70E-03	5.13E+04
Chlorobenzene	108-90-7	1.5	0.1	0.15	0.434	0.284	0.150	7.30E-02	8.70E-06	5.83E-03	1.00E-08	10	15	15	1.80E-04	0.10	1.80E-01	2.04E+02
Chloroform	67-66-03	1.5	0.1	0.15	0.434	0.284	0.150	1.04E-01	1.00E-05	8.31E-03	1.00E-08	10	15	15	1.80E-04	0.07	1.60E-01	5.60E+01
DDT	50-29-3	1.5	0.1	0.15	0.434	0.284	0.150	1.37E-02	4.95E-06	1.09E-03	1.00E-08	10	15	15	1.80E-04	0.51	2.20E43	2.37E+05
1,2-Dichlorobenzene	95-50-1	1.5	0.1	0.15	0.434	0.284	0.150	6.90E-02	7.90E-06	5.51E-03	1.00E-08	10	15	15	1.00E-04	0.10	8.60E-02	3.76E+02
1,4-Dichlorobenzene	106-46-7	1.5	0.1	0.15	0.434	0.284	0.150	6.90E-02	7.90E-06	5.51E-03	1.00E-08	10	15	15	1.80E-04	0.10	1.20E-01	5.16E+02
1,1-Dichloroethane	75-34-3	1.5	0.1	0.15	0.434	0.284	0.150	7.42E-02	1.04E-05	5.93E-03	1.00E-08	10	15	15	1.80E-04	0.09	2.40E41	5.20E+01
1,2-Dichloroethane	107-06-2	1.5	0.1	0.15	0.434	0.284	0.150	1.04E-01	9.90E-06	8.31E-03	1.00E-08	10	15	15	1.80E-04	0.07	5.20E-02	3.80E+01
1,1-Dichloroethylene	75-35 -4	1.5	0.1	0.15	0.434	0.284	0.150	9.00E-02	1.04E-05	7.19E-03	1.00E-08	10	15	15	1.80E-04	0.08	1.00E+00	6.50E+01
1,2-Dichloropropane	78-87-5	1.5	0.1	0.15	0.434	0.284	0.150	7.82E-02	8.73E-06	6.25E-03	1.00E-08	10	15	15	1.80E-04	0.09	1.20E-01	4.70E+01
1,3-Dichloropropene	542-75-6	1.5	0.1	0.15	0.434	0.284	0.150	6.26E-02	1.00E-05	5.00E-03	1.00E-08	10	15	15	1.80E-04	0.11	1.20E-01	2.60E+01
Dieldrin	60-57-1	1.5	0.1	0.15	0.434	0.284	0.150	1.25E-02	4.74E4-6	9.99E-04	1.00E-08	10	15	15	1.80E-04	0.56	1.10E-04	1.09E+04
Ethylbenzene	100-41-4	1.5	0.1	0.15	0.434	0.284	0.150	7.50E-02	7.80E-06	5.99E-03	1.00E-08	10	15	15	1.80E-04	0.09	3.20E-01	2.21E+02
Heptachlor	76-44-8	1.5	0.1	0.15	0.434	0.284	0.150	1.12E-02	5.69E-06	8.95E-04	1.00E-08	10	15	15	1.80E-04	0.62	2.40E-02	6.81E+03
Heptachlor epoxide	1024-57-3	1.5	0.1	0.15	0.434	0.284	0.150	1.22E-02	4.68E-06	9.75E-04	1.00E-08	10	15	15	1.80E-04	0.57	3.40E-04	7.24E+03
Hexachloro-1,3-butadiene	87-68-3	1.5	0.1	0.15	0.434	0.284	0.150	5.61E-02	6.16E-06	4.48E-03	1.00E-08	10	15	15	1.80E-04	0.12	9.80E-01	6.99E+03
Hexachlorobenzene	118-74-1	1.5	0.1	0.15	0.434	0.284	0.150	5.42E-02	5.91E-06	4.33E-03	1.00E-08	10	15	15	1.80E-04	0.13	220E-02	3.75E+04
HCH-alpha(alpha-BHC)	319-84-6	1.5	0.1	0.15	0.434	0.284	0.150	1.76E-02	5.57E-06	1.41E-03	1.00E-08	10	15	15	1.80E-04	0.39	2.80E-04	1.76E+03
HCH-beta(beta-BHC)	319-85-7	1.5	0.1	0.15	0.434	0.284	0.150	1.76E-02	5.57E-06	1.41E-03	1.00E-08	10	15	15	1.80E-04	0.39	1.40E-05	2.28E+03
Hexachlorocyclopentadiene	77-47-4	1.5	0.1	0.15	0.434	0.284	0.150	1.61E-02	7.21E-06	1.29E-03	1.00E-08	10	15	15	1.80E-04	0.43	7.10E-01	9.59E+03
Hexachloroethane	67-72-1	1.5	0.1	0.15	0.434	0.284	0.150	2.49E-03	6.80E-06	1.99E-04	1.00E-08	10	15	15	1.80E-04	2.79	1.50E-01	1.83E+03
Methyl bromide	74-83-9	1.5	0.1	0.15	0.434	0.284	0.150	7.28E-02	1.21E-05	5.82E-03	1.00E-08	10	15	15	1.80E-04	0.10	5.80E-01	9.00E+00
Methylene chloride	75-09-2	1.5	0.1	0.15	0.434	0.284	0.150	1.01E-01	1.17E-05	8.07E-03	1.00E-08	10	15	15	1.80E-04	0.07	9.70E-02	1.60E+01
Nitrobenzene	98-95-3	1.5	0.1	0.15	0.434	0.284	0.150	7.60E-02	8.60E-06	6.07E-03	1.00E-08	10	15	15	1.80E-04	0.09	8.40E-04	1.31E+02
Styrene	100-42-5	1.5	0.1	0.15	0.434	0.284	0.150	7.10E-02	8.00E-06	5.67E-03	1.00E-08	10	15	15	1.80E-04	0.10	1.40E-01	9.12E+02
1,1,2,2-Tetrachloroethane	79-34-5	1.5	0.1	0.15	0.434	0.284	0.150	7.10E-02	7.90E-06	5.67E-03	1.00E-08	10	15	15	1.80E-04	0.10	1.50E-02	7.90E+01
Tetrachloroethylene	127-18-4	1.5	0.1	0.15	0.434	0.284	0.150	7.20E-02	8.20E-06	5.75E-03	1.00E-08	10	15	15	1.80E-04	0.10	7.10E-01	3.00E+02
Toluene	108-88-3	1.5	0.1	0.15	0.434	0.284	0.150	8.70E-02	8.60E-06	6.95E-03	1.00E-08	10	15	15	1.80E-04	0.08	2.50E-01	1.31E+02
Toxaphene	8001-35-2	1.5	0.1	0.15	0.434	0.284	0.150	1.16E-02	4.34E-06	9.27E-04	1.00E-08	10	15	15	1.80E-04	0.60	1.40E-04	5.01E+02
1,2,4-Trichlorobenzene	120-82-1	1.5	0.1	0.15	0.434	0.284	0.150	3.00E-02	8.23E-06	2.40E-03	1.00E-08	10	15	15	1.80E-04	0.23	1.10E-01	1.54E+03
1,1,1-Trichloroethane	71-55-6	1.5	0.1	0.15	0.434	0.284	0.150	7.80E-02	8.80E-06	6.23E-03	1.00E-08	10	15	15	1.80E-04	0.09	7.60E-01	9.90E+01
1,1,2-Trichloroethane	79-00-5	1.5	0.1	0.15	0.434	0.284	0.150	7.80E-02	8.80E-06	6.23E-03	1.00E-08	10	15	15	1.80E-04	0. 09	4.10E-02	7.60E+01
Trichloroethylene	79-01-6	1.5	0.1	0.15	0.434	0.284	0.150	7.90E-02	9.10E-06	6.31E-03	1.00E-08	10	15	15	1.80E-04	0.09	4.30E-01	9.40E+01
2,4,6-Trichlorophenol	88-06-2	1.5	0.1	0.15	0.434	0.284	0.150	3.14E-02	6.36E-06	2.51E-03	1.00E-08	10	15	15	1.80E-04	0.22	1.70E-04	2.83E+02
Vinyl acetate	108-05-4	1.5	0.1	0.15	0.434	0.284	0.150	8.50E-02	9.20E-06	6.79E-03	1.00E-08	10	15	15	1.80E-04	0.08	2.30E-02	5.00E+00
Vinyl chloride	75-01-4	1.5	0.1	0.15	0.434	0.284	0.150	1.06E-01	1.23E-05	8.47E-03	1 00E-08	10	15	15	1.80E-04	0.07	3.50E+00	1.10E+01

NA = not appilcable

^{a} = SSL based on C_{sat}

COMPARISON OF INDOOR AND OUTDOOR INHALATION SSLs FOR VOLATILE CONTAMINANTS

Chemical	Soil organic carbon fraction, f_{oc} (unitless)	Soil-water partition coefficient K_4 (cm^3/g)	Initial soil conc., C_r (mg/kg)	Source vapor conc., C_{source} (g/cm^3)	Floor-wall seam perimeter, X_{crack} (cm)	Crack depth below grade, Z_{crack} (cm)	Crack radius, r_{crack} (cm)	Average vapor flow rate into bldg. Q_{soil} (cm^3/s)	Source-bldg. separation at t=0, L_t^o (cm)	Indoor ψ	Area of base-ment, A_s (cm^2)	Bldg. foundation thick-nesses, L_{crack} (cm)	Crack effective diffusion coeffi-cient, D_{crack} (cm^2/s)	Crack-to-total area ratio, η	Area of crack, A_{crack} (cm^2)	Indoor β	Buiilding ventilation rate, $Q_{building}$ (cm^3/s)	Depth to source lower boundary, ΔH_c (cm)	Exposure duration, τ (sec)
Aldrin	0.006	2.90E+02	1.00E+00	1.45E-05	3400	200	4.06	2.59	15	4.52E-11	1.38E+06	15	1.05E-03	0.01	1.38E+04	3.85E+01	2.90E+04	200	9.46E+08
Benzene	0.006	3.42E-01	1.00E+00	4.55E-01	3400	200	4.06	2.59	15	9.37E-06	1.38E+06	15	6.95E-03	0.01	1.38E+04	2.48E+02	2.90E+04	200	9.46E+08
Bis(2-chloroethyl)ether	0.006	4.56E-01	1.00E+00	1.58E-03	3400	200	4.06	2.59	15	2.59E-08	1.38E+06	15	5.53E-03	0.01	1.38E+04	1.98E+02	2.90E+04	200	9.46E+08
Bromoform	0.006	7.56E-01	1.00E+00	2.90E-02	3400	200	4.06	2.59	15	1.02E-07	1.38E+06	15	1.19E-03	0.01	1.38E+04	4.34E+01	2.90E+04	200	9.46E+08
Carbon disulfide	0.006	3.12E-01	1.00E+00	1.02E+00	3400	200	4.06	2.59	15	2.51E-05	1.38E+06	15	8.31E-03	0.01	1.38E+04	2.97E+02	2.90E+04	200	9.46E+08
Carbon tetrachloride	0.006	9.84E-01	1.00E+00	9.15E-01	3400	200	4.06	2.59	15	1.69E-05	1.38E+06	15	6.23E-03	0.01	1.38E+04	2.23E+02	2.90E+04	200	9.46E+08
Chlordane	0.006	3.08E+02	1.00E+00	8.77E-06	3400	200	4.06	2.59	15	2.45E-11	1.38E+06	15	9.43E-04	0.01	1.38E+04	3.46E+01	2.90E+04	200	9.46E+08
Chlorobenzene	0.006	1.22E+00	1.00E+00	1.33E-01	3400	200	4.06	2.59	15	2.29E-06	1.38E+06	15	5.83E-03	0.01	1.38E+04	2.09E+02	2.90E+04	200	9.46E+08
Chloroform	0.005	3.36E-01	1.00E+00	3.43E-01	3400	200	4.06	2.59	15	8.45E-06	1.38E+06	15	8.31E-03	0.01	1.38E+04	2.97E+02	2.90E+04	200	9.46E+08
DDT	0.006	1.42E+03	1.00E+00	1.55E-06	3400	200	4.06	2.59	15	5.02E-12	1.38E+06	15	1.09E-03	0.01	1.38E+04	4.00E+01	2.90E+04	200	9.46E+08
1,2-Dichlorobenzene	0.006	2.26E+00	1.00E+00	3.63E-02	3400	200	4.06	2.59	15	5.92E-07	1.38E+06	15	5.51E-03	0.01	1.38E+04	1.97E+02	2.90E+04	200	9.46E+08
1,4-Dichlorobenzene	0.006	3.10E+00	1.00E+00	3.73E-02	3400	200	4.06	2.59	15	6.09E-07	1.38E+06	15	5.51E-03	0.01	1.38E+04	1.97E+02	2.90E+04	200	9.46E+08
1,1-Dichloroethane	0.006	3.12E-01	1.00E+00	5.25E-01	3400	200	4.06	2.59	15	9.22E-06	1.38E+06	15	5.93E-03	0.01	1.38E+04	2.12E+02	2.90E+04	200	9.46E+08
1,2-Dichloroethane	0.006	2.28E-01	1.00E+00	1.54E-01	3400	200	4.06	2.59	15	3.79E-06	1.38E+06	15	8.31E-03	0.01	1.38E+04	2.97E+02	2.90E+04	200	9.46E+08
1,1-Dichloroethylene	0.006	3.90E-01	1.00E+00	1.47E+00	3400	200	4.06	2.59	15	3.14E-05	1.38E+06	15	7.19E-03	0.01	1.38E+04	2.57E+02	2.90E+04	200	9.46E+08
1,2-Dichloropropane	0.006	2.82E-01	1.00E+00	2.97E-01	3400	200	4.06	2.59	15	5.49E-06	1.38E+06	15	6.25E-03	0.01	1.38E+04	2.23E+02	2.90E+04	200	9.46E+08
1,3-Dichloropropene	0.006	1.56E-01	1.00E+00	4.31E-01	3400	200	4.06	2.59	15	6.38E-06	1.38E+06	15	5.00E-03	0.01	1.38E+04	1.79E+02	2.90E+04	200	9.46E+08
Dieldrin	0.006	6.54E+01	1.00E+00	1.68E-06	3400	200	4.06	2.59	15	4.97E-12	1.38E+06	15	9.99E-04	0.01	1.38E+04	3.66E+01	2.90E+04	200	9.46E+08
Ethylbenzene	0.006	1.33E+00	1.00E+00	2.15E-01	3400	200	4.06	2.59	15	3.82E-06	1.38E+06	15	5.99E-03	001	1.38E+04	2.14E+02	2.90E+04	200	9.46E+08
Heptachlor	0.006	4.09E+01	1.00E+00	5.86E-04	3400	200	4.06	2.59	15	1.55E-09	1.38E+06	15	8.95E-04	001	1.38E+04	3.29E+01	2.90E+04	200	9.46E+08
Heptachlor epoxide	0.006	4.34E+01	1.00E+00`	7.81E-06	3400	200	4.06	2.59	15	2.26E-11	1.38E+06	15	9.75E-04	0.01	1.38E+04	3.57E+01	2.90E+04	200	9.46E+08
Hexachloro-1,3-butadiene	0.006	4.19E+01	1.00E+00	2.32E-02	3400	200	4.06	2.59	15	3.08E-07	1.38E+06	15	4.48E-03	0.01	1.38E+04	1.61E+02	2.90E+04	200	9.46E+08
Hexachlorobenzene	0.006	2.25E+02	1.00E+00	9.77E-05	3400	200	4.06	2.59	15	1.25E-09	1.38E+06	15	4.33E-03	0.01	1.38E+04	1.55E+02	2.90E+04	200	9.46E+08
HCH-alpha(alpha-BHC)	0.006	1.06E+01	1.00E+00	2.63E-05	3400	200	4.06	2.59	15	1.09E-10	1.38E+06	15	1.41E-03	001	1.38E+04	5.11E+01	2.90E+04	200	9.46E+08
HCH-beta(beta-BHC)	0.006	1.37E+01	1.00E+00	1.02E-06	3400	200	4.06	2.59	15	4.23E-12	1.38E+06	15	1.41E-03	0.01	1.38E+04	5.11E+01	2.90E+04	200	9.46E+08
Hexachlorocyclopentadiene	0.006	5.75E+01	1.00E+00	1.23E-02	3400	200	4.06	2.59	15	4.69E-08	1.38E+06	15	1.29E-03	0.01	1.38E+04	4.68E+01	2.90E+04	200	9.46E+08
Hexachloroethane	0.006	1.10E+01	1.00E+00	1.35E-02	3400	200	4.06	2.59	15	7.96E-09	1.38E+06	15	1.99E-04	0.01	1 38E+04	8.08E+00	2.90E+04	200	9.46E+08
Methyl bromide	0.006	5.40E-02	1.00E+00	2.20E+00	3400	200	4.06	2.59	15	3.79E-05	1.38E+06	15	5.82E-03	0.01	1.38E+04	2.08E+02	2.90E+04	200	9.46E+08
Methylene chloride	0.006	9.60E-02	1.00E+00	4.53E-01	3400	200	4.06	2.59	15	1.08E-05	1.38E+06	15	8.07E-03	0.01	1.38E+04	2.88E+02	2.90E+04	200	9.46E+08
Nitrobenzene	0.006	7.86E-01	1.00E+00	9.48E-04	3400	200	4.06	2.59	15	1.71E-08	1.38E+06	15	6.07E-03	0 01	1 38E+04	2.17E+02	2.90E+04	200	9.46E+08
Styrene	0.006	5.47E+00	1.00E+00	2.50E-02	3400	200	4.06	2.59	15	4.20E-07	1.38E+06	15	5.67E-03	0.01	1.38E+04	2.03E+02	2.90E+04	200	9.46E+08
1,1,2,2-Tetrachloroethane	0.006	4.74E-01	1.00E+00	2.60E-02	3400	200	4.06	2.59	15	4.37E-07	1.38E+06	15	5.67E-03	0.01	1.38E+04	2.03E+02	2.90E+04	200	9.46E+08
Tetrachloroethylene	0.006	1.80E+00	1.00E+00	3.49E-01	3400	200	4.06	2.59	15	5.95E-06	1.38E+06	15	5.75E-03	0.01	1.38E+04	2.06E+02	2.90E+04	200	9.46E+08
Toluene	0.006	7.86E-01	1.00E+00	2.68E-01	3400	200	4.06	2.59	15	5.52E-06	1.38E+06	15	6.95E-03	0.01	1.38E+04	2.48E+02	2.90E+04	200	9.46E+08
Toxaphene	0.006	3.01E+00	1.00E+00	4.51E-05	3400	200	4.06	2.59	15	1.24E-10	1.38E+06	15	9.27E-04	0.01	1.38E+04	3.40E+01	2.90E+04	200	9.46E+08
1,2,4-Trichlorobenzene	0.006	9.24E+00	1.00E+00	1.18E-02	3400	200	4.06	2.59	15	8.35E-08	1.38E+06	15	2.40E-03	0.01	1.38E+04	8.63E+01	2.90E+04	200	9.46E+08
1,1,1-Trichloroethane	0.006	5.94E-01	1.00E+00	9.07E-01	3400	200	4.06	2.59	15	1.68E-05	1.38E+06	15	6.23E-03	0.01	1.38E+04	2.23E+02	2.90E+04	200	9.46E+08
1,1,2-Trichloroethane	0.006	4.56E-01	1.00E+00	7.27E-02	3400	200	4.06	2.59	15	1.34E-06	1.38E+06	15	6.23E-03	0.01	1.38E+04	2.23E+02	2.90E+04	200	9.46E+08
Trichloroethylene	0.006	5.64E-01	1.00E+00	5.77E-01	3400	200	4.06	2.59	15	1.08E-05	1.38E+06	15	6.31E-03	0.01	1.38E+04	2.26E+02	2.90E+04	200	9.46E+08
2,4,6-Trichlorophenol	0.006	1.70E+00	1.00E+00	9.45E-05	3400	200	4.06	2.59	15	7.03E-10	1.38E+06	15	2.51E-03	0.01	1.38E+04	9.03E+01	2.90E+04	200	9.46E+08
Vinyl acetate	0.006	3.00E-02	1.00E+00	1.71E-01	3400	200	4.06	2.59	15	3.45E-06	1.38E+06	15	6.79E-03	0.01	1.38E+04	2.43E+02	2.90E+04	200	9.46E+08
Vinyl chloride	0.006	6.60E-02	1.00E+00	4.22E+00	3400	200	4.06	2.59	15	1.06E-04	1.38E+06	15	8.47E-03	0.01	1.38E+04	3.02E+02	2.90E+04	200	9.46E+08

NA = not appilcable

[a] = SSL based on C_{sat}

COMPARISON OF INDOOR AND OUTDOOR INHALATION SSLs FOR VOLATILE CONTAMINANTS

Chemical	Infinite source indoor attenuation coefficient, α (unitless)	Finite source indoor attenuation coefficient, α (unitless)	Time for source depletion, Indoor τ_D (sec)	Exposure duration > time for depletion (yes/no)	Infinite source bldg. conc., $C_{building}$ (kg/m^3)	Finite source bldg. conc., $C_{building}$ (kg/m^3)	Infinite source indoor volatilization factor VF_{indoor} (m^3/kg)	Finite source indoor volatilization factor VF_{indoor} (m^3/kg)	Unit risk factor, URF $(\mu g/m^3)^{-1}$	Reference conc., RfC (mg/m^3)	Infinite source indoor SSL, carcinogen (mg/kg)	Infinite source indoor SSL, non-carcinogen (mg/kg)	Finite source indoor SSL, carcinogen (mg/kg)	Finite source indoor SSL, non-carcinogen (mg/kg)	Infinite soure risk-based indoor SSL, (mg/kg)	Finite soure risk-based indoor SSL, (mg/kg)	Outdoor apparent diffusion coefficient, α (cm^2/s)	Outdoor volalitization factor, $VF_{outdoor}$ (m^3/kg)
Aldrin	9.32E-05	8.68E-05	1.33E+13	no	1.35E-06	1.26E-06	7.42E+05	7.97E+05	4.90E-03	NA	3.69E-01	NA	3.96E-01	NA	3.69E-.01	3.96E-01	1.99E-09	9.84E+05
Benzene	2.65E-04	8.32E-05	3.63E+08	yes	1.20E-01	1.51E-02	8.30E+00	6.63E+01	8.30E-06	NA	2.43E-03	NA	1.94E-02	NA	2.43E-03	1.94E-02	5.82E-04	1.82E+03
Bis(2-chloroethyl)ether	2.21E-04	8.87E-05	1.05E+11	no	3.50E-04	1.40E-04	2.86E+03	7.13E+03	3.30E-04	NA	2.11E-02	NA	5.26E-02	NA	2.11E-02	5.26E-02	1.39E-06	3.72E+04
Bromoform	9.59E-05	8.50E-05	6.51E+09	no	2.79E-03	2.47E-03	3.59E+02	4.05E+02	1.10E-06	NA	7.94E-01	NA	8.96E-01	NA	7.94E-01	8.96E-01	5.13E-06	1.94E+04
Carbon disulfide	3.07E-04	7.93E-05	1.61E+08	yes	3.13E-01	1.51E-02	3.20E+00	6.63E+01	NA	1.00E-02	NA	3.33E-02	NA	6.91E-01	3.33E-02	6.91E-01	1.80E-03	1.03E+03
Carbon tetrachloride	2.43E-04	7.78E-05	1.81E+08	yes	2.22E-01	1.51E-02	4.50E+00	6.63E+01	1.50E-05	NA	7.31E-04	NA	1.08E-02	NA	7.31E-04	1.08E-02	9.90E-04	1.39E+03
Chlordane	9.11E-05	8.66E-05	2.24E+13	no-	7.99E-07	7.59E-07	1.25E+06	1.32E+06	6.00E-05	NA	5.08E+01	NA	5.34E+01	NA	5.08E+01	5.34E+01	1.08E-09	1.34E+06
Chlorobenzene	2.30E-04	8.66E-05	1.25E+09	no	3.05E-02	1.15E-02	3.28E+01	8.71E+01	NA	2.00E-02	NA	6.83E-01	NA	1.82E+00	6.83E-01	1.82E+00	1.12E-04	4.15E+03
Chloroform	3.07E-04	8.51E-05	4.79E+08	yes	1.05E-01	1.51E-02	9.49E+00	6.63E+01	2.30E-05	NA	1.00E-03	NA	7.01E-03	NA	1 00E-03	7.01E-03	5.15E-04	1.93E+03
DDT	9.40E-05	8.69E-05	1.24E+14	no	1.45E-07	1.34E-07	6.88E+06	7.44E+06	9.70E-05	NA	1.73E+02	NA	1.87E+02	NA	1.73E+02	1.87E+02	2.21E-10	2.95E+06
1,2-Dichlorobenzene	2.20E-04	8.81E-05	4.59E+09	no	7.99E-03	3.19E-03	1.25E+02	3.13E+02	NA	2.00E-01	NA	2.61E+01	NA	6.53E+01	2.61E+01	6.53E+01	2.74E-05	8.38E+03
1,4-Dichlorobenzene	2.20E-04	8.81E-05	4.46E+09	no	8.22E-03	3.28E-03	1.22E+02	3.05E+02	NA	8.00E-01	NA	1.02E+02	NA	2.54E+02	1.02E+02	2.54E+02	2.78E-05	8.32E+03
1,1-Dichloroethane	2.33E-04	8.15E-05	3.16E+08	yes	1.22E-01	1.51E-02	8.17E+00	6.63E+01	NA	5.00E-01	NA	4.26E+00	NA	3.46E+01	4.26E+00	3.46E+01	5.94E-04	1.80E+03
1,2-Dichloroethane	3.07E-04	8.71E-05	1.07E+09	no	4.73E-02	1.34E-02	2.12E+01	7.46E+01	2.60E-05	NA	1.98E-03	NA	6.98E-03	NA	1.98E-03	6.98E-03	2.47E-04	2.79E+03
1,1-Dichloroethylene	2.72E-04	7.47E-05	1.12E+08	yes	4.01E-01	1.51E-02	2.49E+00	6.63E+01	5.00E-05	NA	1.21E-04	NA	3.23E-03	NA	1.21E-04	3.23E-03	2.40E-03	8.95E+02
1,2-Dichloropropane	2.43E-04	8.46E-05	5.59E+08	yes	7.21E-02	1.51E-02	1.39E+01	6.63E+01	NA	4.00E-03	NA	5.79E-02	NA	2.76E-01	5.79E-02	2.76E-01	3.46E-04	2.36E+03
1,3-Dichloropropene	2.05E-04	8.16E-05	3.88E+08	yes	8.82E-02	1.51E-02	1.13E+01	6.63E+01	3.70E-05	2.00E-02	7.46E-04	2.37E-01	4.36E-03	1.38E+00	7.46E-04	4.36E-03	5.01E-04	1.96E+03
Dieldrin	9.21E-05	8.67E-05	1.16E+14	no	1.55E-07	1.46E-07	6.47E+06	6.87E+06	4.60E-03	NA	3.42E+00	NA	3.63E+00	NA	3.42E+00	3.63E+00	2.19E-10	2.97E+06
Ethylbenzene	2.35E-04	8.55E-05	7.71E+08	yes	5.06E-02	1.51E-02	1.97E+01	6.63E+01	NA	1.00E+00	NA	2.06E+01	NA	6.91E+01	2.06E+01	6.91E+01	1.88E-04	3.20E+03
Heptachlor	9.02E-05	8.64E-05	3.39E+11	no	5.29E-05	5.06E-05	1.89E+04	1.98E+04	1.30E-03	NA	3.54E-02	NA	3.70E-02	NA	3.54E-02	3.70E-02	6.84E-08	1.68E+05
Heptachlor epoxide	9.16E-05	8.67E-05	2.50E+13	no	7.16E-07	6.77E-07	1.40E+06	1.48E+06	2.60E-03	NA	1.31E+00	NA	1.38E+00	NA	1.31E+00	1.38E+00	9.93E-10	1.39E+06
Hexachloro-1,3-butadiene	1.89E-04	8.81E-05	7.23E+09	no	4.38E-03	2.04E-03	2.28E+02	4.89E+02	2.20E-05	NA	2.52E-02	NA	5.41E-02	NA	2.52E-02	5.41E-02	1.36E-05	1.19E+04
Hexachlorobenzene	1.84E-04	8.86E-05	1.72E+12	no	1.80E-05	8.66E-06	5.55E+04	1.16E+05	4.60E-04	NA	2.94E-01	NA	6.11E-01	NA	2.94E-01	6.11E-01	5.51E-08	1.87E+05
HCH-alpha(alpha-BHC)	1.01E-04	8.74E-05	7.03E+12	no	2.65E-06	2.30E-06	3.78E+05	4.36E+05	1.80E-03	NA	5.11E-01	NA	5.89E-01	NA	5.11E-01	5.89E-01	4.85E-09	6.29E+05
HCH-beta(beta-BHC)	1.01E-04	8.74E-05	1.82E+14	no	1.02E-07	8.88E-08	9.76E+06	1.13E+07	5.30E-04	NA	4.48E+01	NA	5.17E+01	NA	4.48E+01	5.17E+01	1.87E-10	3.20E+06
Hexachlorocyclopentadiene	9.80E-05	8.64E-05	1.52E+10	no	1.20E-03	1.06E-03	8.30E+02	9.42E+02	NA	7.00E-05	NA	6.06E-02	NA	6.88E-02	6.06E-02	6.88E-02	2.07E-06	3.05E+04
Hexachloroethane	7.81E-05	7.41E-05	2.47E+10	no	1.05E-03	1.00E-03	9.48E+02	1.00E+03	4.00E-06	NA	5.77E-01	NA	6.08E-01	NA	5.77E-01	6.08E-01	3.54E-07	7.37E+04
Methyl bromide	2.30E-04	6.75E-05	7.55E+07	yes	5.05E-01	1.51E-02	1.98E+00	6.63E+01	NA	5.00E-03	NA	1.03E-02	NA	3.46E-01	1.03E-02	3.46E-01	8.13E-03	4.86E+02
Methylene chloride	3.00E-04	8.40EE-05	3.63E+08	yes	1.36E-01	1.51E-02	7.38E+00	6.63E+01	4.70E-07	3.00E+00	3.82E-02	2.31E+01	3.43E-01	2.07E+02	3.82E-02	3.43E-01	1.06E-03	1.35E+03
Nitrobenzene	2.38E-04	8.87E-05	1.75E+11	no	2.25E-04	8.41E-05	4.44E+03	1.19E+04	NA	2.00E-03	NA	9.26E+00	NA	2.48E+01	9.26E+00	2.48E+01	8.45E-07	4.77E+04
Styrene	2.25E-04	8.83E-05	6.65E+09	no	5.64E-03	2.21E-03	1.77E+02	4.53E+02	NA	1.00E+00	NA	1.85E+02	NA	4.72E+02	1.85E+02	4.72E+02	1.89E-05	1.01E+04
1,1,2,2-Tetrachloroethane	2.25E-04	8.83E-05	6.39E+09	no	5.86E-03	2.30E-03	1.71E+02	4.36E+02	5.80E-05	NA	7.16E-03	NA	1.83E-02	NA	7.16E-03	1.83E-02	2.34E-05	9.07E+03
Tetrachloroethylene	2.28E-04	8.35E-05	4.76E+08	yes	7.95E-02	1.51E-02	1.26E+01	6.63E+01	5.80E-07	NA	5.28E-02	NA	2.78E-01	NA	5.28E-02	2.78E-01	2.95E-04	2.55E+03
Toluene	2.65E-04	8.53E-05	6.16E+08	yes	7.10E-02	1.51E-02	1.41E+01	6.63E+01	NA	4.00E-01	NA	5.88E+00	NA	2.76E+01	5.88E+00	2.76E+01	2.88E-04	2.59E+03
Toxaphene	9.08E-05	8.65E-05	4.38E+12	no	4.09E-06	3.90E-06	2.44E+05	2.56E+05	3.20E-04	NA	1.86E+00	NA	1.95E+00	NA	1.86E+00	1.95E+00	5.62E-09	5.85E+05
1,2,4-Trichlorobenzene	1.27E-04	8.77E-05	1.49E+10	no	1.49E-03	1.03E-03	6.70E+02	9.71E+02	NA	9.00E-03	NA	6.29E+00	NA	9.11E+00	6.29E+00	9.11E+00	3.72E-06	2.28E+04
1,1,1-Trichloroethane	2.43E-04	7.79E-05	1.83E+08	yes	2.20E-01	1.51E-02	4.54E+00	6.63E+01	NA	1.00E+00	NA	4.74E+00	NA	6.91E+01	4.74E+00	6.91E+01	1.04E-03	1.36E+03
1,1,2-Trichloroethane	2.43E-04	8.76E-05	2.28E+09	no	1.76E-02	6.37E-03	5.67E+01	1.57E+02	1.60E-05	NA	8.62E-03	NA	2.39E-02	NA	8.62E-03	2.39E-02	7.30E-05	5.13E+03
Trichloroethylene	2.45E-04	8.13E-05	2.87E+08	yes	1.41E-01	1.51E-02	7.07E+00	6.63E+01	1.70E-06	NA	1.01E-02	NA	9.49E-02	NA	1.01E-02	9.49E-02	6.27E-04	1.75E+03
2,4,6-Trichlorophenol	1.30E-04	8.82E-05	1.84E+12	no	1.23E-05	8.34E-06	8.13E+04	1.20E+05	3.10E-06	NA	6.38E+01	NA	9.42E+01	NA	6.38E+01	9.42E+01	3.27E-08	2.43E+05
Vinyl acetate	2.60E-04	8.65E-05	9.65E+08	no	4.45E-02	1.48E-02	2.25E+01	6.76E+01	NA	2.00E-01	NA	4.69E+00	NA	1.41E+01	4.69E+00	1.41E+01	6.78E-04	1.68E+03
Vinyl chloride	3.12E-04	6.38E-05	3.89E+07	yes	1.32E+00	1.51E-02	7.59E-01	6.63E+01	8.40E-05	NA	2.20E-05	NA	1.92E-03	NA	2.20E-05	1.92E-03	5.85E-02	1.81E+02

NA = not appilcable
[a] = SSL based on C_{sat}

COMPARISON OF INDOOR AND OUTDOOR INHALATION SSLs FOR VOLATILE CONTAMINANTS

Chemical	Outdoor SSL, carcinogen (mg/kg)	Outdoor SSL, non-carcinogen (mg/kg)	Risk-based outdoor SSL (mg/kg)	Pure component solubility, S (mg/L)	Soil saturation conc., C_{sat} (mg/kg)	Indoor SSL, infinite source (mg/kg)	Indoor SSL, finite source (mg/kg)	Outdoor SSL, infinite source (mg/kg)
Aldrin	4.89E-01	NA	4.89E-01	7.84E-02	2.28E+01	0.4	0.4	0.5
Benzene	5.33E-01	NA	5.33E-01	1.78E+03	8.61E+02	0.002	0.02	0.5
Bis(2-chloroethyl)ether	2.74E-01	NA	2.74E-01	1.18E+04	6.56E+03	0.02	0.05	0.3
Bromoform	4.29E+01	NA	4.29E+01	3.21E+03	2.76E+03	0.8	0.9	43
Carbon disulfide	NA	1.08E+01	1.08E+01	2.67E+03	1.36E+03	0.03	0.7	11
Carbon tetrachloride	2.26E-01	NA	2.26E-01	7.92E+02	1.04E+03	0.0007	0.01	0.2
Chlordane	5.42E+01	NA	5.42E+01	2.19E-01	6.74E+01	51	53	54
Chlorobenzene	NA	8.66E+01	8.66E+01	4.09E+02	5.55E+02	0.7	2	87
Chloroform	2.04E-01	NA	2.04E-01	7.96E+03	3.71E+03	0.001	0.007	0.2
DDT	7.41E+01	NA	7.41E+01	3.41E-03	4.85E+00	5[a]	5[a]	5[a]
1,2-Dichlorobenzene	NA	1.75E+03	1.75E+03	1.25E+02	2.97E+02	26	65	297[a]
1,4-Dichlorobenzene	NA	6.94E+03	6.94E+03	7.30E+01	2.35E+02	102	235	235[a]
1,1-Dichloroethane	NA	9.39E+02	9.39E+02	5.16E+03	2.36E+03	4	35	939
1,2-Dichloroethane	2.61E-01	NA	2.61E-01	8.31E+03	2.81E+03	0.002	0.007	0.3
1,1-Dichloroethylene	4.36E-02	NA	4.36E-02	3.00E+03	2.04E+03	0.0001	0.003	0.04
1,2-Dichloropropane	NA	9.83E+00	9.83E+00	2.68E+03	1.08E+03	0.06	0.3	10
1,3-Dichloropropene	1.29E-01	4.09E+01	1.29E-01	1.55E+03	4.32E+02	0.0007	0.004	0.1
Dieldrin	1.57E+00	NA	1.57E+00	1.87E-01	1.22E+01	3	4	2
Ethylbenzene	NA	3.33E+03	3.33E+03	1.73E+02	2.57E+02	21	69	257[a]
Heptachlor	3.14E-01	NA	3.14E-01	2.73E-01	1.12E+01	0.04	0.04	0.3
Heptachlor epoxide	1.30E+00	NA	1.30E+00	2.68E-01	1.17E+01	1	1	1
Hexachloro-1,3-butadiene	1.31E+00	NA	1.31E+00	2.54E+00	1.07E+02	0.03	0.05	1
Hexachlorobenzene	9.88E-01	NA	9.88E-01	8.62E-03	1.94E+00	0.3	0.6	1
HCH-alpha(alpha-BHC)	8.51E-01	NA	8.51E-01	2.40E+00	2.56E+01	0.5	0.6	0.9
HCH-beta(beta-BHC)	1.47E+01	NA	1.47E+01	5.42E-01	7.47E+00	7[a]	7[a]	7[a]
Hexachlorocyclopentadiene	NA	2.23E+00	2.23E+00	1.53E+00	8.84E+01	0.06	0.07	2
Hexachloroethane	4.48E+01	NA	4.48E+01	4.08E+01	4.53E+02	0.6	0.6	45
Methyl bromide	NA	2.54E+00	2.54E+00	1.45E+04	3.83E+03	0.01	0.3	3
Methylene chloride	6.97E+00	4.21E+03	6.97E+00	1.74E+04	3.73E+03	0.04	0.3	7
Nitrobenzene	NA	9.95E+01	9.95E+01	1.92E+03	1.70E+03	9	25	100
Styrene	NA	1.05E+04	1.05E+04	2.57E+02	1.44E+03	185	472	1439
1,1,2,2-Tetrachloroethane	3.81E-01	NA	3.81E-01	3.07E+03	1.77E+03	0.007	0.02	0.4
Tetrachloroethylene	1.07E+01	NA	1.07E+01	2.32E+02	4.72E+02	0.05	0.3	11
Toluene	NA	1.08E+03	1.08E+03	5.58E+02	5.21E+02	6	28	521[a]
Toxaphene	4.45E+00	NA	4.45E+00	6.79E-01	2.11E+00	2	2	2[a]
1,2,4-Trichlorobenzene	NA	2.14E+02	2.14E+02	3.07E+01	2.87E+02	6	9	214
1,1,1-Trichloroethane	NA	1.42E+03	1.42E+03	1.17E+03	9.80E+02	5	69	980[a]
1,1,2-Trichloroethane	7.81E-01	NA	7.81E-01	4.40E+03	2.48E+03	0.009	0.02	1
Trichloroethylene	2.51E+00	NA	2.51E+00	1.18E+03	8.80E+02	0.01	0.09	3
2,4,6-Trichlorophenol	1.90E+02	NA	1.90E+02	7.53E+02	1.35E+03	64	94	190
Vinyl acetate	NA	3.51E+02	3.51E+02	2.24E+04	3.01E+03	5	14	351
Vinyl chloride	5.25E-03	NA	5.25E-03	2.73E+03	2.26E+03	0.00002	0.002	0.01

NA = not appilcable

[a] = SSL based on C_{sat}

APPENDIX I

SSL Simulation Results

APPENDIX I

SSL Simulation Results

Section 4.3.3 contains a complete description of the simulation setup and parameters. The following notation is used in the tables of this appendix.

C = the number of specimens per composite
N = the number of composite samples chemically analyzed
MU = the assumed true site mean (= 0.5 SSL or 2 SSL)
CV = the assumed true value of the site coefficient of variation, (i.e. the true site standard deviation divided by the true site mean MU)
MIX = the proportion of the site which is uncontaminated

The remaining variables give the estimated probability of deciding to investigate further (PDIF) for a given method and simulation distribution. The variable names indicate the method of testing (Mx = Max test, C = Chen test, L = Land test) and the type of probability distribution used to generate values for the contaminated part of the EA (L = lognormal, G = gamma, W = Weibull).

MxL, MxG, MxW = PDIF for Max rule applied to lognormal, gamma or Weibull data

C40L, C40G, C40W = PDIF for Chen test at the nominal .40 significance level applied to lognormal, gamma or Weibull data

C30L, C30G, C30W = PDIF for Chen test at the nominal .30 significance level applied to lognormal, gamma or Weibull data

C20L, C20G, C20W = PDIF for Chen test at the nominal .20 significance level applied to lognormal, gamma or Weibull data

C1OL, C1OG, C1OW= PDIF for Chen test at the nominal .10 significance level applied to lognormal, gamma or Weibull data

C05L, C05G, C05W = PDIF for Chen test at the nominal .05 significance level applied to lognormal, gamma or Weibull data

COlL, CO1G, CO1W = PDIF for Chen test at the nominal .01 significance level applied to lognormal, gamma or Weibull data

LfL, LfG, LfW = PDIF for Land test of the flipped null hypothesis at the nominal .10 significance level applied to lognormal, gamma or Weibull data

LoL, LoG, LoW = PDIF for Land test of the original null hypothesis at the nominal .05 significance level applied to lognormal, gamma or Weibull data.

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=1 N=4 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.124	.314	.246	.161	.087	.042	.016	.099	.835	.195	.350	.276	.195	.088	.043	.011	.172	.975	.176	.360	.286	.209	.104	.042	.009	.151	.945
0.5	.50	.192	.371	.295	.182	.089	.039	.016	.297	.937	.194	.347	.270	.170	.072	.028	.013	.257	.931	.194	.373	.294	.197	.086	.039	.017	.265	.929
2.0	.00	.750	.974	.960	.926	.858	.759	.426	.873	.972	.757	.874	.838	.775	.650	.494	.188	.742	.991	.760	.903	.870	.808	.707	.551	.240	.768	.988
2.0	.50	.848	.863	.816	.745	.569	.361	.132	.703	.947	.792	.813	.774	.699	.540	.334	.106	.659	.925	.825	.839	.799	.729	.589	.370	.117	.686	.952

C=1 N=4 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.140	.296	.227	.150	.073	.036	.007	.088	.887	.255	.338	.277	.198	.106	.046	.009	.182	.965	.219	.315	.261	.169	.084	.033	.006	.143	.961
0.5	.50	.213	.320	.240	.167	.080	.036	.010	.214	.932	.273	.343	.273	.191	.084	.031	.007	.201	.905	.241	.330	.261	.167	.075	.032	.009	.214	.902
0.5	.75	.343	.387	.298	.193	.067	.021	.004	.241	.673	.366	.407	.302	.170	.061	.023	.008	.205	.680	.377	.414	.305	.175	.055	.016	.003	.215	.676
2.0	.00	.700	.919	.890	.838	.733	.593	.260	.765	.964	.676	.740	.698	.645	.493	.341	.072	.624	.988	.695	.809	.770	.716	.596	.433	.138	.663	.995
2.0	.50	.753	.813	.766	.688	.524	.339	.112	.680	.941	.694	.712	.675	.625	.466	.291	.072	.522	.926	.713	.747	.698	.620	.481	.295	.073	.585	.938
2.0	.75	.699	.698	.689	.657	.456	.176	.028	.433	.704	.675	.673	.658	.615	.430	.161	.030	.406	.681	.669	.664	.642	.596	.442	.175	.027	.425	.694

C=1 N=4 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.157	.266	.203	.138	.072	.026	.002	.088	.900	.256	.317	.257	.197	.089	.034	.004	.183	.944	.225	.306	.236	.168	.078	.028	.005	.145	.948
0.5	.50	.212	.296	.227	.165	.085	.038	.007	.186	.927	.267	.324	.260	.187	.093	.033	.003	.194	.868	.264	.310	.263	.189	.091	.032	.006	.191	.896
0.5	.85	.459	.445	.357	.208	.060	.014	.001	.103	.490	.449	.437	.350	.215	.063	.015	.006	.117	.486	.441	.432	.350	.213	.064	.012	.005	.120	.499
2.0	.00	.642	.857	.816	.764	.648	.512	.192	.672	.962	.620	.668	.623	.562	.423	.266	.044	.526	.972	.624	.718	.671	.605	.469	.331	.073	.558	.986
2.0	.50	.692	.752	.699	.620	.468	.312	.089	.617	.930	.613	.630	.592	.537	.404	.219	.040	.496	.885	.635	.672	.627	.567	.412	.233	.036	.530	.918
2.0	.85	.481	.481	.481	.480	.438	.082	.009	.421	.481	.474	.474	.474	.474	.425	.096	.008	.406	.474	.473	.473	.470	.464	.419	.091	.011	.404	.474

C=1 N=4 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.180	.280	.234	.163	.091	.034	.002	.119	.912	.263	.291	.238	.178	.093	.030	.004	.164	.859	.226	.275	.226	.163	.087	.029	.005	.142	.950
0.5	.50	.206	.277	.225	.158	.074	.029	.002	.170	.941	.277	.297	.244	.179	.075	.028	.002	.142	.764	.270	.302	.253	.181	.087	.024	.003	.163	.872
0.5	.85	.366	.364	.289	.207	.090	.023	.001	.135	.501	.316	.309	.265	.198	.075	.015	.002	.105	.450	.359	.353	.306	.235	.098	.028	.003	.133	.480
2.0	.00	.632	.820	.778	.724	.593	.429	.143	.631	.965	.566	.589	.552	.502	.377	.225	.030	.455	.921	.581	.657	.615	.558	.430	.280	.048	.514	.986
2.0	.50	.631	.683	.637	.558	.434	.277	.068	.574	.939	.531	.555	.501	.447	.329	.179	.024	.388	.860	.591	.616	.588	.530	.395	.242	.038	.489	.905
2.0	.85	.457	.457	.456	.438	.336	.106	.005	.314	.459	.451	.450	.444	.422	.356	.123	.002	.348	.465	.471	.468	.455	.435	.353	.138	.005	.348	.491

C=1 N=4 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.187	.267	.221	.152	.085	.035	.002	.104	.905	.231	.252	.203	.149	.078	.019	.003	.124	.784	.226	.259	.214	.163	.080	.034	.002	.137	.945
0.5	.50	.210	.262	.217	.154	.082	.029	.002	.151	.897	.268	.273	.242	.186	.098	.022	.002	.145	.722	.231	.266	.214	.170	.079	.026	.004	.141	.860
0.5	.90	.312	.306	.275	.199	.070	.021	.002	.071	.336	.301	.299	.266	.222	.101	.018	.000	.094	.341	.299	.293	.266	.216	.096	.023	.001	.099	.348
2.0	.00	.616	.791	.746	.674	.555	.397	.103	.580	.962	.489	.509	.466	.416	.311	.179	.017	.361	.862	.558	.631	.587	.509	.398	.247	.037	.477	.983
2.0	.50	.607	.659	.601	.532	.403	.270	.058	.521	.945	.512	.516	.492	.445	.338	.199	.014	.376	.819	.524	.549	.506	.448	.331	.190	.023	.410	.891
2.0	.90	.346	.346	.346	.346	.310	.131	.002	.307	.346	.363	.363	.362	.356	.321	.111	.000	.311	.364	.328	.328	.327	.324	.291	.120	.004	.289	.331

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=1 N=4 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.173	.241	.203	.141	.061	.024	.003	.091	.920	.255	.265	.234	.177	.093	.029	.002	.141	.727	.194	.213	.178	.131	.068	.025	.001	.105	.910
0.5	.50	.198	.239	.190	.142	.072	.027	.001	.135	.916	.232	.235	.191	.146	.078	.027	.001	.106	.643	.235	.254	.215	.147	.074	.023	.000	.125	.822
0.5	.90	.273	.268	.235	.184	.078	.012	.000	.089	.329	.280	.269	.242	.196	.111	.032	.003	.115	.375	.240	.234	.207	.155	.082	.020	.000	.092	.324
2.0	.00	.594	.750	.708	.632	.502	.387	.104	.534	.963	.443	.450	.426	.387	.294	.162	.009	.333	.753	.511	.579	.526	.466	.342	.213	.018	.445	.979
2.0	.50	.590	.655	.596	.501	.385	.239	.039	.513	.942	.453	.459	.424	.380	.283	.150	.009	.315	.751	.505	.517	.486	.427	.318	.166	.017	.380	.878
2.0	.90	.354	.354	.351	.340	.305	.123	.001	.296	.355	.330	.330	.325	.314	.277	.132	.004	.270	.340	.330	.326	.320	.301	.254	.145	.000	.254	.353

C=1 N=6 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.183	.338	.252	.180	.089	.039	.005	.099	.636	.250	.353	.270	.173	.098	.047	.006	.172	.953	.218	.357	.279	.184	.061	.027	.005	.128	.916
0.5	.50	.233	.367	.285	.206	.100	.055	.014	.320	.981	.276	.371	.298	.206	.104	.049	.007	.300	.971	.320	.418	.303	.208	.107	.045	.007	.304	.965
2.0	.00	.860	.986	.979	.971	.939	.896	.658	.945	.946	.873	.928	.902	.861	.789	.677	.356	.843	.992	.882	.956	.940	.908	.841	.733	.417	.878	.992
2.0	.50	.931	.924	.901	.844	.722	.565	.242	.799	.992	.926	.899	.868	.830	.730	.573	.235	.781	.980	.920	.891	.869	.821	.705	.543	.213	.768	.988

C=1 N=6 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.220	.301	.237	.168	.081	.032	.004	.099	.728	.348	.348	.280	.189	.100	.039	.005	.182	.957	.317	.346	.276	.202	.101	.040	.004	.157	.947
0.5	.50	.260	.304	.253	.176	.085	.034	.005	.223	.965	.366	.369	.281	.183	.088	.034	.002	.209	.931	.387	.372	.289	.217	.114	.039	.003	.243	.958
0.5	.75	.459	.385	.293	.197	.083	.038	.007	.188	.844	.486	.395	.296	.199	.082	.030	.003	.179	.833	.504	.393	.298	.187	.068	.023	.003	.172	.809
2.0	.00	.816	.960	.946	.917	.849	.760	.481	.855	.947	.822	.832	.802	.752	.630	.497	.167	.721	.993	.831	.887	.849	.805	.689	.539	.229	.758	.990
2.0	.50	.891	.891	.842	.777	.633	.497	.189	.732	.989	.837	.818	.786	.718	.609	.453	.155	.657	.966	.846	.834	.787	.713	.607	.450	.147	.675	.980
2.0	.75	.819	.796	.769	.697	.506	.353	.068	.461	.824	.804	.777	.747	.696	.518	.360	.058	.478	.812	.786	.768	.738	.665	.473	.313	.058	.423	.804

C=1 N=6 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.267	.292	.241	.163	.095	.047	.004	.105	.796	.356	.324	.254	.172	.088	.044	.005	.162	.921	.286	.297	.243	.162	.090	.040	.005	.138	.942
0.5	.50	.312	.333	.266	.190	.092	.035	.004	.219	.956	.371	.329	.252	.179	.073	.034	.002	.152	.892	.373	.340	.263	.183	.089	.035	.004	.178	.919
0.5	.85	.591	.409	.300	.194	.082	.031	.003	.154	.631	.597	.434	.311	.200	.085	.027	.000	.154	.637	.559	.434	.318	.203	.073	.019	.001	.156	.618
2.0	.00	.804	.932	.905	.868	.791	.681	.340	.801	.947	.759	.745	.705	.649	.521	.362	.086	.585	.980	.781	.815	.772	.715	.599	.474	.150	.664	.990
2.0	.50	.827	.834	.789	.724	.591	.435	.151	.710	.973	.765	.734	.700	.636	.520	.367	.076	.552	.951	.795	.756	.708	.641	.512	.370	.107	.576	.963
2.0	.85	.628	.628	.628	.621	.456	.221	.014	.226	.628	.596	.596	.596	.586	.431	.223	.019	.226	.596	.650	.649	.646	.629	.470	.230	.020	.232	.651

C=1 N=6 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.249	.282	.230	.159	.083	.034	.001	.091	.808	.380	.327	.275	.211	.101	.036	.003	.155	.854	.336	.322	.254	.191	.100	.039	.004	.149	.941
0.5	.50	.305	.296	.235	.164	.083	.031	.008	.173	.950	.393	.337	.274	.208	.100	.040	.001	.161	.844	.337	.296	.239	.183	.094	.035	.007	.144	.877
0.5	.85	.495	.377	.290	.188	.072	.024	.003	.118	.647	.486	.397	.329	.228	.099	.033	.005	.132	.647	.460	.371	.306	.211	.081	.027	.001	.112	.624
2.0	.00	.797	.899	.865	.833	.745	.595	.261	.760	.956	.705	.669	.621	.560	.444	.307	.060	.487	.947	.720	.752	.707	.652	.517	.391	.112	.595	.985
2.0	.50	.778	.780	.740	.670	.544	.379	.114	.644	.980	.690	.646	.602	.537	.429	.287	.049	.443	.892	.704	.676	.634	.557	.442	.312	.068	.477	.952
2.0	.85	.637	.623	.607	.556	.403	.215	.023	.230	.638	.611	.585	.564	.524	.403	.209	.029	.239	.627	.583	.560	.536	.500	.406	.203	.023	.224	.604

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=1 N=6 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.240	.251	.203	.140	.079	.028	.002	.082	.833	.361	.309	.271	.201	.102	.034	.002	.130	.785	.296	.265	.216	.160	.085	.037	.003	.117	.927
0.5	.50	.289	.271	.212	.154	.080	.040	.003	.137	.931	.369	.307	.240	.164	.087	.037	.003	.103	.784	.340	.287	.237	.176	.099	.040	.002	.126	.854
0.5	.90	.407	.326	.258	.185	.093	.032	.001	.091	.441	.417	.340	.290	.202	.079	.037	.002	.086	.460	.403	.357	.311	.223	.085	.033	.000	.084	.457
2.0	.00	.771	.870	.832	.777	.680	.544	.217	.706	.958	.616	.586	.529	.470	.373	.234	.034	.371	.873	.714	.727	.684	.614	.489	.344	.080	.562	.987
2.0	.50	.756	.744	.687	.629	.513	.354	.099	.598	.980	.647	.602	.564	.508	.410	.259	.038	.389	.851	.672	.636	.596	.535	.433	.270	.058	.463	.936
2.0	.90	.442	.440	.440	.433	.354	.123	.014	.123	.442	.449	.445	.442	.428	.350	.140	.014	.141	.451	.472	.468	.459	.448	.375	.143	.009	.144	.476

C=1 N=6 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.246	.255	.200	.131	.062	.023	.004	.084	.839	.342	.275	.229	.181	.092	.028	.001	.099	.725	.289	.268	.216	.153	.088	.034	.002	.121	.883
0.5	.50	.299	.271	.213	.153	.086	.037	.002	.134	.922	.315	.269	.220	.160	.084	.020	.000	.087	.691	.325	.275	.226	.173	.080	.035	.001	.112	.818
0.5	.90	.396	.324	.269	.196	.082	.022	.000	.065	.453	.400	.340	.296	.211	.099	.041	.001	.078	.497	.350	.301	.254	.196	.078	.030	.003	.058	.438
2.0	.00	.723	.847	.797	.724	.600	.470	.179	.626	.956	.559	.523	.494	.450	.334	.214	.023	.323	.821	.675	.679	.634	.568	.457	.317	.057	.519	.982
2.0	.50	.745	.735	.683	.609	.482	.342	.093	.597	.968	.576	.532	.495	.429	.334	.200	.023	.299	.792	.623	.574	.531	.468	.348	.236	.032	.380	.906
2.0	.90	.477	.472	.464	.439	.337	.140	.007	.145	.479	.471	.449	.437	.415	.335	.164	.013	.168	.489	.446	.428	.411	.390	.326	.160	.013	.175	.473

C=1 N=9 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.286	.335	.274	.205	.112	.057	.010	.112	.452	.363	.390	.293	.202	.089	.043	.006	.216	.937	.336	.375	.287	.188	.092	.036	.008	.168	.880
0.5	.50	.365	.380	.298	.203	.108	.050	.014	.380	.984	.420	.411	.301	.213	.103	.046	.009	.336	.980	.416	.392	.290	.201	.095	.046	.008	.335	.972
2.0	.00	.948	.999	.999	.995	.989	.965	.891	.987	.950	.955	.973	.963	.936	.887	.815	.577	.933	.999	.957	.985	.974	.965	.927	.855	.648	.950	.994
2.0	.50	.983	.956	.940	.904	.820	.719	.449	.856	.995	.978	.954	.930	.900	.817	.697	.430	.841	.994	.973	.955	.936	.907	.828	.713	.403	.863	.991

C=1 N=9 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.312	.314	.247	.173	.101	.049	.005	.110	.592	.472	.369	.297	.199	.096	.034	.005	.206	.934	.397	.317	.239	.159	.087	.048	.009	.151	.907
0.5	.50	.425	.366	.289	.205	.092	.045	.007	.287	.962	.496	.384	.285	.199	.102	.045	.010	.250	.940	.495	.385	.301	.220	.112	.058	.010	.255	.940
0.5	.75	.629	.418	.307	.215	.107	.053	.008	.198	.840	.642	.417	.324	.208	.102	.051	.005	.187	.841	.656	.396	.306	.209	.102	.037	.003	.193	.840
2.0	.00	.913	.987	.983	.974	.955	.910	.714	.953	.948	.913	.897	.864	.828	.742	.619	.341	.808	.997	.933	.950	.930	.905	.826	.727	.409	.872	.989
2.0	.50	.951	.923	.892	.842	.756	.630	.338	.816	.989	.930	.908	.884	.844	.710	.576	.271	.743	.987	.938	.888	.860	.790	.696	.558	.267	.720	.986
2.0	.75	.918	.873	.826	.752	.615	.464	.138	.456	.920	.925	.872	.842	.761	.642	.469	.170	.472	.927	.920	.866	.838	.764	.609	.465	.170	.470	.923

C=1 N=9 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.364	.323	.256	.179	.092	.044	.006	.097	.667	.477	.346	.283	.196	.090	.046	.004	.166	.864	.435	.350	.287	.199	.103	.049	.003	.159	.906
0.5	.50	.416	.315	.250	.172	.096	.042	.006	.216	.957	.525	.377	.297	.209	.101	.045	.007	.184	.862	.473	.341	.270	.188	.107	.049	.004	.179	.871
0.5	.85	.706	.384	.280	.186	.083	.027	.002	.118	.744	.737	.407	.315	.197	.093	.036	.004	.118	.754	.719	.406	.307	.185	.081	.025	.001	.100	.746
2.0	.00	.910	.980	.970	.954	.905	.846	.593	.912	.952	.867	.821	.782	.725	.623	.486	.191	.656	.983	.886	.892	.861	.811	.712	.601	.316	.788	.992
2.0	.50	.931	.900	.868	.823	.731	.607	.322	.790	.990	.888	.823	.788	.729	.628	.489	.179	.629	.961	.902	.834	.798	.738	.615	.489	.203	.649	.976
2.0	.85	.743	.741	.731	.681	.458	.367	.073	.364	.743	.764	.762	.750	.686	.432	.355	.064	.351	.764	.782	.773	.760	.708	.459	.370	.090	.366	.782

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=1 N=9 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.354	.292	.218	.153	.074	.030	.006	.093	.729	.494	.338	.276	.205	.115	.049	.008	.144	.817	.426	.313	.256	.172	.079	.038	.003	.133	.850
0.5	.50	.443	.313	.239	.166	.091	.041	.003	.191	.948	.507	.337	.265	.173	.082	.029	.002	.121	.801	.464	.330	.264	.194	.105	.047	.004	.156	.854
0.5	.85	.615	.391	.310	.203	.103	.040	.003	.101	.686	.604	.363	.284	.200	.085	.030	.002	.080	.660	.609	.379	.284	.187	.083	.032	.005	.085	.671
2.0	.00	.888	.953	.930	.895	.840	.739	.438	.834	.937	.851	.785	.731	.676	.548	.399	.099	.537	.955	.863	.856	.823	.777	.684	.560	.226	.751	.988
2.0	.50	.900	.878	.848	.803	.693	.570	.232	.767	.983	.833	.744	.707	.644	.519	.368	.111	.485	.927	.855	.805	.761	.700	.597	.446	.166	.610	.958
2.0	.85	.763	.726	.690	.618	.467	.306	.069	.287	.764	.753	.708	.682	.622	.479	.315	.089	.303	.764	.736	.692	.660	.612	.476	.306	.077	.299	.744

C=1 N=9 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.353	.271	.222	.158	.085	.046	.002	.096	.742	.474	.323	.271	.198	.092	.046	.006	.112	.728	.418	.293	.249	.190	.106	.051	.004	.127	.835
0.5	.50	.427	.319	.259	.186	.103	.038	.005	.179	.911	.471	.329	.265	.194	.094	.053	.002	.102	.701	.427	.293	.241	.175	.080	.040	.003	.119	.790
0.5	.90	.572	.350	.276	.201	.099	.036	.002	.053	.595	.537	.353	.288	.199	.097	.040	.003	.058	.560	.553	.383	.322	.214	.108	.043	.003	.059	.584
2.0	.00	.880	.927	.902	.876	.800	.699	.385	.819	.951	.766	.690	.652	.604	.483	.333	.083	.434	.896	.836	.796	.748	.693	.572	.435	.171	.639	.982
2.0	.50	.885	.841	.795	.739	.606	.503	.198	.688	.983	.779	.699	.659	.612	.493	.335	.087	.409	.873	.819	.721	.683	.618	.506	.369	.097	.507	.954
2.0	.90	.624	.620	.614	.577	.390	.195	.030	.189	.624	.610	.592	.581	.560	.401	.209	.056	.203	.611	.620	.594	.573	.537	.424	.213	.041	.204	.624

C=1 N=9 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.385	.301	.230	.168	.097	.042	.005	.108	.755	.475	.315	.255	.182	.099	.043	.003	.079	.673	.408	.267	.211	.154	.076	.038	.002	.118	.798
0.5	.50	.431	.307	.252	.181	.097	.033	.003	.152	.876	.444	.323	.270	.215	.116	.040	.004	.089	.628	.431	.299	.239	.174	.088	.034	.005	.098	.747
0.5	.90	.520	.326	.267	.197	.099	.042	.007	.057	.546	.483	.324	.267	.191	.095	.037	.003	.044	.527	.471	.321	.275	.181	.077	.030	.001	.038	.510
2.0	.00	.858	.895	.862	.809	.723	.619	.292	.740	.952	.730	.640	.596	.535	.429	.280	.056	.348	.845	.836	.774	.729	.665	.558	.410	.143	.607	.977
2.0	.50	.864	.808	.774	.719	.610	.475	.173	.690	.982	.709	.608	.568	.520	.399	.257	.046	.308	.822	.797	.733	.674	.603	.488	.330	.089	.477	.924
2.0	.90	.636	.609	.582	.523	.395	.223	.040	.205	.636	.594	.544	.523	.484	.385	.201	.031	.171	.601	.588	.544	.523	.478	.373	.201	.035	.179	.594

C=1 N=12 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.350	.368	.276	.206	.102	.054	.014	.109	.280	.480	.386	.296	.207	.097	.045	.004	.241	.922	.438	.353	.276	.189	.096	.056	.008	.185	.821
0.5	.50	.450	.397	.311	.209	.122	.057	.009	.441	.989	.494	.398	.312	.208	.094	.048	.014	.398	.974	.507	.396	.313	.223	.107	.052	.013	.386	.975
2.0	.00	.985	1.00	1.00	1.00	.999	.993	.962	.998	.955	.989	.993	.984	.971	.939	.906	.751	.967	.998	.987	.996	.990	.986	.972	.948	.808	.980	.990
2.0	.50	.998	.977	.965	.950	.904	.822	.598	.905	.998	.995	.981	.963	.948	.897	.815	.571	.902	.996	.992	.971	.948	.926	.877	.800	.560	.876	.994

C=1 N=12 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.390	.330	.273	.186	.084	.041	.004	.094	.439	.576	.383	.300	.199	.101	.043	.006	.223	.949	.524	.377	.305	.214	.124	.059	.008	.204	.919
0.5	.50	.496	.367	.281	.189	.093	.046	.008	.313	.964	.593	.351	.264	.178	.085	.046	.009	.231	.943	.590	.393	.321	.225	.119	.057	.012	.285	.940
0.5	.75	.738	.396	.290	.181	.100	.057	.008	.171	.856	.747	.414	.320	.201	.090	.041	.011	.186	.822	.741	.402	.302	.198	.085	.047	.007	.181	.809
2.0	.00	.967	.997	.995	.993	.977	.959	.865	.978	.946	.977	.952	.927	.899	.821	.746	.480	.890	.999	.977	.978	.965	.946	.895	.840	.595	.937	.998
2.0	.50	.988	.967	.949	.918	.852	.763	.500	.867	1.00	.971	.933	.910	.878	.778	.682	.399	.786	.991	.981	.947	.920	.880	.793	.684	.402	.811	.995
2.0	.75	.963	.907	.875	.821	.702	.580	.301	.565	.905	.972	.928	.900	.840	.724	.598	.305	.575	.929	.954	.900	.866	.818	.706	.558	.281	.542	.907

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=1 N=12 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.435	.296	.223	.159	.084	.038	.005	.089	.520	.627	.375	.293	.201	.092	.040	.006	.176	.902	.530	.340	.273	.190	.088	.038	.005	.164	.898
0.5	.50	.492	.305	.234	.175	.083	.041	.006	.227	.942	.623	.384	.287	.195	.087	.042	.007	.159	.878	.614	.377	.285	.197	.093	.045	.005	.187	.910
0.5	.85	.833	.413	.312	.194	.104	.036	.003	.092	.596	.802	.411	.308	.216	.097	.046	.009	.091	.558	.814	.387	.290	.195	.086	.037	.003	.086	.539
2.0	.00	.968	.991	.984	.982	.959	.921	.720	.963	.956	.939	.879	.852	.803	.703	.583	.289	.742	.991	.965	.948	.919	.877	.816	.709	.406	.873	.996
2.0	.50	.969	.940	.914	.877	.799	.686	.395	.844	.995	.951	.882	.850	.795	.691	.577	.257	.684	.976	.954	.894	.860	.824	.736	.624	.307	.731	.983
2.0	.85	.859	.844	.812	.720	.544	.406	.116	.250	.842	.851	.835	.807	.715	.568	.455	.120	.264	.830	.856	.829	.798	.730	.549	.438	.134	.255	.822

C=1 N=12 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.429	.311	.239	.162	.079	.042	.005	.092	.612	.600	.365	.283	.197	.099	.043	.004	.119	.806	.547	.337	.258	.190	.090	.047	.006	.145	.870
0.5	.50	.510	.322	.253	.187	.109	.043	.005	.217	.930	.610	.365	.300	.211	.114	.059	.005	.148	.778	.565	.355	.269	.192	.093	.048	.006	.149	.842
0.5	.85	.728	.381	.290	.205	.117	.056	.012	.088	.593	.707	.358	.283	.198	.107	.052	.004	.089	.540	.713	.404	.315	.225	.118	.053	.004	.090	.591
2.0	.00	.933	.972	.959	.932	.900	.843	.605	.909	.932	.925	.821	.784	.724	.608	.492	.183	.587	.964	.933	.901	.873	.832	.754	.634	.310	.808	.992
2.0	.50	.955	.917	.883	.843	.748	.634	.318	.797	.991	.909	.826	.786	.719	.599	.458	.167	.520	.943	.912	.852	.814	.752	.634	.510	.227	.637	.972
2.0	.85	.844	.769	.718	.631	.511	.364	.124	.252	.760	.852	.786	.745	.680	.535	.378	.130	.267	.784	.820	.755	.716	.657	.529	.380	.119	.250	.762

C=1 N=12 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.437	.307	.237	.174	.095	.044	.005	.111	.660	.608	.360	.294	.214	.108	.042	.005	.109	.735	.505	.316	.260	.194	.110	.046	.004	.139	.841
0.5	.50	.508	.305	.238	.174	.094	.040	.003	.173	.908	.589	.325	.259	.182	.082	.046	.004	.088	.708	.541	.301	.247	.179	.093	.039	.006	.110	.788
0.5	.90	.680	.377	.299	.196	.085	.037	.001	.033	.409	.666	.388	.304	.204	.100	.050	.004	.055	.424	.632	.386	.316	.235	.121	.047	.005	.049	.434
2.0	.00	.940	.957	.934	.912	.857	.777	.522	.863	.952	.870	.760	.712	.648	.529	.394	.134	.445	.929	.918	.870	.838	.792	.677	.563	.238	.747	.991
2.0	.50	.945	.900	.863	.809	.715	.596	.284	.765	.989	.866	.749	.690	.627	.506	.359	.108	.398	.889	.886	.783	.737	.668	.572	.438	.176	.561	.963
2.0	.90	.723	.710	.684	.628	.420	.295	.083	.147	.703	.709	.685	.656	.598	.439	.283	.092	.158	.681	.708	.672	.654	.605	.445	.288	.091	.166	.670

C=1 N=12 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.470	.290	.226	.169	.090	.043	.005	.103	.699	.559	.317	.261	.197	.107	.049	.005	.081	.640	.525	.328	.273	.201	.099	.047	.004	.116	.848
0.5	.50	.495	.313	.263	.173	.098	.043	.002	.152	.904	.563	.319	.260	.182	.108	.043	.004	.080	.632	.559	.340	.274	.197	.097	.045	.006	.107	.785
0.5	.90	.638	.351	.289	.193	.094	.051	.007	.052	.425	.605	.365	.304	.204	.095	.043	.004	.040	.442	.585	.343	.282	.196	.093	.049	.002	.046	.412
2.0	.00	.942	.950	.926	.899	.824	.740	.471	.838	.955	.830	.705	.667	.605	.490	.347	.093	.374	.861	.883	.803	.760	.710	.618	.497	.181	.668	.983
2.0	.50	.930	.849	.819	.769	.673	.561	.227	.736	.985	.817	.689	.640	.586	.481	.317	.087	.325	.830	.880	.774	.735	.678	.555	.415	.136	.508	.945
2.0	.90	.713	.672	.640	.575	.425	.286	.074	.151	.666	.710	.652	.621	.569	.437	.257	.051	.139	.654	.706	.647	.611	.568	.443	.252	.061	.148	.643

C=1 N=16 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.438	.354	.279	.202	.102	.053	.007	.092	.161	.565	.393	.307	.216	.100	.058	.012	.293	.900	.542	.371	.287	.196	.111	.054	.010	.223	.801
0.5	.50	.535	.387	.303	.205	.110	.062	.014	.482	.986	.586	.411	.291	.200	.111	.052	.004	.459	.976	.595	.400	.292	.204	.103	.062	.007	.447	.978
2.0	.00	.996	1.00	1.00	1.00	1.00	1.00	.997	1.00	.957	.994	.995	.992	.989	.975	.956	.872	.989	.999	.993	.997	.996	.990	.983	.973	.924	.988	.995
2.0	.50	1.00	.990	.982	.973	.950	.910	.761	.945	1.00	.999	.988	.982	.959	.925	.875	.714	.932	.998	.998	.987	.976	.962	.928	.885	.734	.922	.999

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=1 N=16 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.502	.331	.258	.173	.099	.061	.007	.103	.291	.682	.401	.319	.219	.113	.057	.009	.279	.937	.628	.378	.304	.209	.108	.050	.008	.217	.870
0.5	.50	.596	.379	.291	.202	.112	.058	.011	.371	.966	.736	.394	.296	.213	.092	.041	.006	.276	.935	.691	.400	.308	.205	.100	.047	.009	.290	.950
0.5	.75	.804	.401	.314	.229	.098	.051	.007	.197	.805	.809	.389	.308	.206	.093	.046	.004	.173	.783	.849	.404	.300	.218	.103	.038	.005	.187	.794
2.0	.00	.990	.997	.997	.996	.993	.987	.939	.992	.957	.994	.981	.976	.957	.919	.851	.623	.956	.998	.997	.995	.991	.980	.961	.925	.753	.982	1.00
2.0	.50	.997	.984	.975	.957	.920	.850	.659	.925	.999	.992	.971	.952	.929	.866	.778	.528	.862	.996	.995	.960	.947	.928	.871	.790	.566	.875	.997
2.0	.75	.992	.950	.927	.886	.805	.697	.404	.599	.946	.987	.950	.920	.873	.789	.672	.413	.563	.928	.987	.941	.917	.876	.781	.690	.394	.607	.924

C=1 N=16 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.541	.327	.265	.188	.110	.047	.009	.112	.420	.700	.375	.298	.204	.106	.057	.009	.195	.872	.636	.335	.252	.179	.094	.044	.006	.170	.868
0.5	.50	.629	.364	.294	.209	.110	.053	.009	.300	.947	.725	.347	.276	.196	.107	.060	.014	.155	.834	.693	.392	.305	.194	.096	.046	.004	.193	.872
0.5	.85	.892	.405	.319	.204	.101	.043	.003	.085	.576	.898	.420	.307	.212	.099	.050	.009	.079	.604	.908	.398	.306	.206	.111	.049	.002	.090	.600
2.0	.00	.984	.994	.991	.985	.978	.962	.849	.978	.953	.979	.922	.905	.864	.785	.688	.425	.813	.992	.980	.971	.955	.940	.897	.837	.581	.935	.998
2.0	.50	.991	.965	.948	.923	.871	.799	.557	.885	.995	.972	.918	.899	.860	.784	.671	.384	.736	.976	.982	.932	.912	.873	.807	.717	.423	.799	.988
2.0	.85	.926	.899	.847	.772	.657	.489	.199	.285	.719	.935	.904	.868	.794	.710	.520	.244	.337	.755	.928	.896	.861	.787	.675	.478	.201	.297	.731

C=1 N=16 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.559	.322	.240	.173	.096	.036	.005	.094	.504	.705	.367	.267	.186	.096	.045	.007	.119	.776	.621	.333	.262	.179	.082	.042	.004	.144	.845
0.5	.50	.618	.330	.268	.181	.087	.039	.006	.226	.924	.716	.375	.289	.210	.113	.052	.008	.128	.729	.680	.358	.281	.200	.107	.054	.007	.160	.822
0.5	.85	.808	.391	.304	.220	.123	.060	.007	.079	.543	.821	.396	.309	.203	.103	.060	.009	.076	.540	.812	.405	.311	.210	.092	.045	.006	.061	.539
2.0	.00	.976	.986	.981	.966	.949	.907	.747	.949	.948	.973	.895	.868	.814	.710	.579	.294	.656	.979	.968	.943	.925	.890	.824	.739	.467	.877	.996
2.0	.50	.982	.948	.929	.899	.831	.732	.457	.860	.995	.962	.874	.848	.790	.682	.550	.257	.596	.952	.967	.902	.868	.822	.733	.627	.338	.732	.974
2.0	.85	.926	.850	.800	.734	.615	.478	.195	.285	.720	.905	.830	.773	.721	.576	.449	.193	.277	.705	.909	.841	.805	.739	.611	.451	.177	.282	.716

C=1 N=16 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.531	.287	.224	.156	.080	.038	.004	.084	.520	.676	.354	.286	.209	.108	.046	.007	.094	.683	.621	.331	.268	.202	.103	.045	.005	.130	.820
0.5	.50	.642	.331	.273	.200	.102	.056	.007	.209	.906	.667	.352	.278	.192	.099	.048	.004	.079	.636	.675	.359	.291	.201	.113	.053	.004	.123	.746
0.5	.90	.787	.387	.302	.211	.097	.044	.004	.033	.415	.760	.390	.303	.197	.097	.048	.004	.034	.419	.750	.381	.288	.212	.114	.052	.012	.045	.399
2.0	.00	.978	.984	.978	.961	.924	.880	.691	.938	.960	.935	.804	.769	.710	.599	.473	.221	.499	.914	.952	.892	.869	.820	.750	.652	.337	.791	.996
2.0	.50	.973	.932	.913	.872	.792	.677	.397	.830	.995	.915	.787	.756	.695	.582	.455	.180	.432	.876	.955	.874	.849	.801	.705	.565	.256	.657	.968
2.0	.90	.803	.772	.728	.655	.506	.380	.128	.190	.504	.799	.744	.714	.639	.485	.357	.125	.168	.493	.813	.758	.725	.665	.510	.360	.111	.167	.524

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=1 N=16 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.543	.306	.249	.184	.112	.056	.003	.108	.576	.652	.327	.262	.190	.095	.038	.003	.058	.576	.629	.311	.264	.173	.086	.035	.002	.108	.771
0.5	.50	.611	.302	.250	.168	.087	.042	.005	.144	.858	.663	.336	.273	.199	.100	.044	.006	.064	.555	.647	.314	.245	.179	.086	.037	.005	.094	.705
0.5	.90	.721	.351	.280	.185	.095	.045	.004	.025	.383	.700	.346	.279	.189	.093	.037	.003	.018	.359	.707	.370	.296	.221	.095	.046	.011	.029	.356
2.0	.00	.973	.980	.966	.944	.900	.841	.598	.905	.957	.897	.753	.709	.649	.535	.399	.127	.372	.866	.954	.857	.820	.766	.682	.574	.275	.722	.987
2.0	.50	.976	.898	.869	.823	.738	.634	.352	.787	.994	.896	.742	.695	.635	.513	.393	.144	.342	.836	.932	.825	.785	.718	.606	.491	.195	.560	.951
2.0	.90	.810	.745	.714	.642	.493	.346	.106	.158	.533	.784	.700	.663	.611	.456	.304	.099	.138	.504	.793	.708	.672	.611	.466	.329	.099	.155	.507

C=4N=4 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.035	.336	.261	.176	.088	.045	.018	.084	.687	.029	.403	.307	.221	.122	.082	.043	.126	.814	.030	.377	.291	.204	.095	.059	.031	.107	.797
0.5	.50	.026	.374	.280	.211	.113	.073	.033	.156	.852	.019	.390	.295	.204	.125	.073	.039	.177	.868	.013	.398	.301	.202	.117	.076	.042	.178	.850
2.0	.00	.835	1.00	1.00	1.00	.997	.991	.890	.997	.960	.857	.994	.988	.984	.966	.924	.674	.977	.983	.840	.996	.994	.993	.980	.946	.739	.983	.976
2.0	.50	.887	.994	.989	.978	.943	.845	.631	.989	.990	.886	.982	.976	.958	.909	.823	.572	.974	.994	.891	.989	.979	.955	.897	.795	.540	.965	.995

C=14N=4 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.070	.331	.255	.188	.100	.059	.029	.106	.753	.089	.383	.292	.183	.103	.058	.020	.136	.931	.072	.381	.288	.195	.104	.054	.015	.126	.871
0.5	.50	.091	.354	.292	.206	.120	.066	.024	.161	.889	.089	.385	.303	.205	.110	.064	.029	.187	.930	.067	.364	.277	.187	.097	.052	.026	.174	.925
0.5	.75	.055	.385	.293	.197	.117	.074	.036	.339	.939	.059	.394	.300	.205	.107	.074	.042	.358	.932	.056	.379	.268	.183	.104	.065	.030	.312	.947
2.0	.00	.788	.999	.997	.993	.983	.964	.762	.983	.966	.820	.964	.952	.931	.860	.737	.436	.905	.994	.821	.983	.979	.966	.923	.858	.568	.939	.982
2.0	.50	.855	.976	.964	.947	.890	.791	.512	.960	.985	.870	.967	.953	.923	.837	.683	.360	.928	.996	.839	.974	.963	.927	.832	.704	.408	.930	.992
2.0	.75	.884	.939	.911	.864	.742	.560	.283	.900	.987	.885	.954	.924	.861	.723	.543	.267	.914	.991	.889	.933	.904	.846	.695	.518	.243	.877	.989

C=4 N=4 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.093	.295	.240	.172	.096	.047	.010	.101	.769	.133	.354	.283	.194	.085	.043	.018	.162	.963	.117	.332	.267	.181	.091	.045	.015	.112	.898
0.5	.50	.102	.319	.241	.172	.097	.050	.021	.144	.918	.136	.362	.260	.180	.094	.050	.015	.201	.967	.128	.342	.255	.170	.078	.038	.016	.153	.956
0.5	.85	.129	.401	.303	.179	.076	.050	.038	.394	.914	.121	.396	.283	.174	.080	.058	.046	.415	.907	.126	.378	.274	.160	.081	.046	.036	.371	.906
2.0	.00	.764	.994	.992	.982	.963	.904	.653	.964	.957	.814	.945	.910	.868	.771	.611	.296	.836	.991	.797	.969	.952	.927	.868	.762	.427	.889	.985
2.0	.50	.832	.966	.959	.935	.846	.735	.422	.928	.991	.808	.915	.883	.832	.720	.573	.268	.842	.988	.810	.925	.902	.855	.754	.610	.279	.857	.993
2.0	.85	.893	.888	.833	.751	.525	.327	.129	.668	.922	.886	.886	.845	.757	.538	.355	.143	.677	.917	.880	.882	.836	.761	.554	.339	.140	.683	.913

C=4 N=4 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.107	.321	.249	.176	.090	.041	.013	.098	.844	.192	.371	.277	.181	.077	.033	.009	.194	.975	.149	.328	.258	.178	.090	.041	.014	.122	.929
0.5	.50	.119	.321	.241	.165	.076	.039	.014	.134	.918	.188	.351	.273	.180	.082	.036	.011	.197	.977	.177	.349	.270	.175	.082	.039	.009	.176	.958
0.5	.85	.195	.364	.279	.187	.087	.036	.010	.328	.927	.211	.404	.317	.212	.096	.052	.017	.351	.918	.212	.368	.298	.209	.084	.037	.016	.327	.920
2.0	.00	.762	.987	.979	.971	.943	.872	.586	.948	.964	.762	.875	.840	.783	.656	.462	.171	.761	.995	.749	.933	.909	.864	.777	.628	.306	.811	.978
2.0	.50	.791	.947	.920	.878	.784	.664	.340	.890	.990	.801	.887	.853	.793	.668	.491	.163	.810	.997	.762	.897	.863	.817	.697	.511	.211	.820	.995
2.0	.85	.819	.826	.782	.710	.549	.355	.121	.668	.928	.824	.833	.796	.731	.568	.342	.111	.690	.929	.828	.842	.797	.738	.552	.332	.109	.696	.936

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=4 N=4 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.116	.279	.220	.154	.082	.038	.008	.091	.834	.242	.376	.295	.196	.090	.033	.008	.219	.975	.171	.303	.246	.174	.082	.038	.008	.126	.932
0.5	.50	.140	.308	.239	.166	.083	.042	.009	.134	.934	.236	.362	.287	.201	.097	.042	.009	.239	.978	.183	.327	.255	.168	.083	.038	.010	.165	.980
0.5	.90	.260	.371	.289	.188	.083	.038	.013	.315	.806	.291	.403	.304	.189	.080	.032	.010	.330	.822	.284	.376	.278	.173	.078	.029	.009	.295	.803
2.0	.00	.749	.979	.974	.952	.902	.829	.517	.909	.970	.712	.808	.763	.697	.573	.406	.125	.712	.992	.728	.903	.871	.834	.715	.568	.241	.770	.983
2.0	.50	.753	.928	.901	.857	.756	.629	.306	.853	.988	.736	.806	.769	.714	.582	.371	.125	.720	.994	.750	.871	.828	.770	.642	.488	.193	.757	.996
2.0	.90	.784	.780	.744	.675	.510	.278	.074	.574	.826	.786	.782	.732	.671	.495	.255	.067	.569	.826	.773	.764	.730	.665	.488	.251	.050	.574	.824

C=4 N=4 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.125	.263	.210	.148	.079	.038	.007	.090	.849	.277	.358	.291	.202	.096	.040	.007	.226	.964	.174	.302	.236	.173	.087	.037	.009	.131	.938
0.5	.50	.162	.303	.240	.173	.085	.039	.008	.146	.945	.251	.339	.261	.182	.082	.034	.007	.205	.957	.233	.336	.286	.198	.108	.043	.010	.192	.969
0.5	.90	.297	.371	.293	.196	.070	.024	.007	.276	.823	.307	.376	.288	.198	.076	.033	.009	.266	.800	.307	.382	.297	.182	.066	.029	.009	.265	.813
2.0	.00	.711	.966	.953	.929	.856	.768	.441	.865	.959	.680	.751	.714	.655	.512	.330	.086	.664	.994	.709	.859	.832	.780	.671	.519	.171	.729	.984
2.0	.50	.737	.907	.871	.825	.728	.559	.238	.814	.990	.699	.753	.704	.640	.519	.319	.075	.657	.981	.690	.798	.765	.699	.573	.410	.134	.713	.992
2.0	.90	.721	.718	.684	.626	.442	.244	.056	.544	.814	.716	.720	.686	.627	.458	.236	.047	.543	.833	.695	.696	.660	.603	.445	.239	.054	.539	.800

C=4 N=6 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.048	.336	.262	.185	.092	.039	.013	.087	.315	.042	.390	.305	.203	.103	.056	.022	.122	.604	.043	.391	.293	.196	.088	.045	.018	.098	.572
0.5	.50	.047	.401	.309	.209	.120	.060	.028	.205	.685	.024	.383	.308	.214	.106	.062	.030	.210	.741	.027	.407	.306	.212	.111	.064	.021	.213	.769
2.0	.00	.928	1.00	1.00	1.00	1.00	.999	.993	1.00	.965	.961	1.00	1.00	1.00	.997	.994	.918	.999	.986	.940	1.00	1.00	1.00	1.00	.993	.931	.998	.981
2.0	.50	.964	.999	.998	.995	.981	.947	.803	.997	.992	.966	.998	.996	.988	.973	.941	.783	.996	.998	.962	.999	.998	.995	.985	.951	.781	.999	.995

C=4 N=6 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.091	.368	.288	.193	.105	.058	.020	.111	.481	.106	.369	.285	.187	.089	.044	.013	.129	.843	.113	.364	.278	.182	.091	.046	.008	.111	.738
0.5	.50	.089	.378	.293	.205	.108	.049	.011	.174	.805	.112	.382	.293	.206	.118	.073	.019	.231	.900	.122	.390	.300	.198	.100	.053	.018	.214	.899
0.5	.75	.075	.390	.298	.209	.114	.066	.026	.457	.944	.090	.398	.311	.207	.101	.054	.022	.434	.951	.088	.409	.303	.194	.100	.051	.022	.446	.960
2.0	.00	.906	1.00	1.00	1.00	.998	.996	.966	.999	.963	.930	.991	.984	.978	.960	.913	.693	.966	.992	.923	.997	.996	.991	.977	.960	.810	.978	.978
2.0	.50	.937	.994	.992	.982	.965	.916	.715	.995	.992	.943	.985	.979	.966	.916	.852	.594	.972	.997	.947	.996	.987	.977	.946	.884	.642	.984	.996
2.0	.75	.952	.967	.951	.924	.848	.753	.429	.941	.998	.960	.973	.960	.942	.879	.770	.431	.953	.999	.964	.971	.960	.931	.851	.741	.408	.941	1.00

C=4 N=6 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.134	.347	.274	.187	.109	.062	.009	.119	.554	.200	.385	.292	.206	.099	.040	.010	.183	.906	.158	.336	.268	.188	.096	.053	.006	.133	.805
0.5	.50	.186	.383	.293	.210	.097	.048	.010	.176	.844	.212	.385	.294	.195	.095	.042	.008	.234	.958	.198	.376	.299	.203	.093	.049	.007	.212	.938
0.5	.85	.175	.363	.264	.163	.087	.050	.023	.406	.970	.178	.389	.292	.204	.091	.043	.014	.435	.975	.196	.418	.308	.203	.107	.048	.019	.445	.968
2.0	.00	.889	.997	.997	.997	.990	.983	.891	.993	.968	.907	.975	.957	.929	.885	.805	.514	.923	.994	.893	.993	.987	.976	.941	.895	.658	.952	.981
2.0	.50	.911	.989	.983	.963	.936	.887	.642	.977	.997	.917	.963	.950	.923	.860	.771	.455	.941	.997	.926	.976	.967	.948	.898	.810	.531	.956	.999
2.0	.85	.980	.941	.913	.854	.710	.534	.204	.837	.984	.953	.913	.885	.834	.685	.517	.186	.818	.972	.974	.944	.914	.869	.744	.565	.204	.854	.983

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further.

C=4 N=6 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.159	.305	.235	.161	.082	.037	.006	.089	.639	.274	.384	.306	.212	.098	.053	.014	.230	.977	.224	.351	.273	.185	.083	.046	.010	.125	.847
0.5	.50	.201	.350	.272	.183	.093	.050	.006	.175	.888	.283	.373	.293	.211	.105	.040	.010	.258	.983	.236	.339	.272	.187	.097	.052	.005	.209	.949
0.5	.85	.270	.399	.307	.204	.102	.045	.012	.394	.972	.290	.366	.281	.182	.071	.033	.007	.338	.969	.308	.386	.308	.197	.087	.040	.012	.360	.963
2.0	.00	.862	.998	.995	.994	.988	.965	.797	.988	.957	.867	.923	.901	.871	.791	.668	.328	.863	.994	.875	.983	.969	.950	.908	.835	.533	.924	.984
2.0	.50	.887	.978	.972	.948	.897	.814	.528	.944	.992	.886	.938	.914	.874	.774	.631	.315	.885	.997	.887	.942	.921	.891	.817	.716	.393	.894	.995
2.0	.85	.924	.901	.878	.812	.668	.523	.202	.791	.978	.917	.896	.863	.805	.684	.526	.195	.774	.979	.923	.898	.872	.822	.700	.544	.198	.786	.980

C=4 N=6 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.182	.332	.260	.195	.110	.048	.007	.122	.687	.316	.359	.280	.193	.106	.051	.008	.221	.984	.254	.354	.279	.207	.104	.046	.011	.168	.896
0.5	.50	.194	.308	.249	.182	.104	.050	.005	.158	.882	.315	.355	.283	.194	.085	.032	.008	.238	.986	.292	.352	.281	.199	.115	.048	.010	.215	.958
0.5	.90	.372	.378	.311	.199	.092	.041	.005	.298	.912	.387	.407	.308	.204	.090	.037	.007	.314	.934	.376	.366	.273	.174	.081	.036	.006	.258	.915
2.0	.00	.852	.993	.989	.982	.970	.933	.738	.970	.959	.843	.884	.851	.799	.692	.531	.234	.808	.994	.854	.953	.939	.914	.862	.764	.434	.883	.981
2.0	.50	.862	.968	.956	.929	.862	.774	.469	.937	.996	.886	.896	.867	.824	.722	.555	.212	.837	.998	.865	.917	.898	.860	.770	.632	.288	.868	.997
2.0	.90	.885	.844	.796	.735	.582	.408	.099	.640	.910	.880	.841	.813	.743	.584	.397	.102	.645	.913	.882	.832	.794	.714	.572	.394	.099	.613	.917

C=4 N=6 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.185	.305	.248	.184	.101	.042	.006	.109	.689	.366	.371	.295	.200	.103	.040	.005	.230	.975	.272	.325	.245	.183	.095	.040	.004	.145	.916
0.5	.50	.208	.318	.239	.175	.087	.035	.008	.157	.899	.355	.380	.307	.210	.102	.047	.007	.258	.980	.302	.342	.275	.191	.084	.039	.004	.181	.969
0.5	.90	.395	.390	.301	.200	.100	.041	.005	.289	.916	.402	.366	.298	.196	.082	.033	.005	.255	.895	.396	.368	.280	.180	.083	.031	.005	.248	.871
2.0	.00	.856	.991	.991	.985	.962	.921	.699	.969	.967	.822	.839	.805	.750	.650	.496	.174	.755	.992	.835	.931	.908	.871	.789	.680	.359	.829	.987
2.0	.50	.856	.956	.941	.910	.839	.743	.398	.915	.990	.844	.850	.820	.777	.655	.495	.170	.768	.994	.828	.889	.855	.803	.698	.583	.259	.819	.999
2.0	.90	.870	.820	.774	.707	.557	.404	.113	.625	.916	.865	.828	.786	.721	.577	.411	.111	.621	.935	.830	.791	.754	.673	.540	.369	.105	.570	.922

C=4 N=9 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.093	.390	.311	.214	.124	.071	.016	.126	.106	.074	.416	.317	.215	.112	.063	.017	.141	.376	.068	.379	.290	.199	.109	.056	.012	.120	.287
0.5	.50	.076	.400	.311	.202	.110	.069	.017	.249	.575	.047	.411	.313	.224	.116	.063	.022	.287	.663	.040	.428	.329	.220	.113	.061	.022	.269	.671
2.0	.00	.981	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.963	.988	1.00	1.00	1.00	.998	.998	.990	.999	.989	.988	1.00	1.00	1.00	1.00	.999	.997	1.00	.987
2.0	.50	.994	1.00	1.00	1.00	.999	.997	.962	1.00	.999	.993	1.00	1.00	1.00	.997	.992	.951	1.00	.998	.990	1.00	1.00	.999	.997	.995	.955	1.00	.998

C=4 N=9 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.153	.364	.281	.201	.111	.053	.009	.109	.239	.179	.390	.290	.206	.095	.053	.014	.165	.744	.188	.384	.311	.218	.093	.055	.014	.125	.571
0.5	.50	.156	.365	.267	.184	.101	.049	.011	.213	.746	.160	.387	.288	.209	.114	.055	.015	.292	.879	.177	.369	.288	.190	.093	.045	.010	.247	.868
0.5	.75	.130	.398	.312	.204	.094	.046	.011	.591	.983	.120	.386	.287	.190	.101	.047	.019	.595	.973	.118	.400	.296	.185	.084	.046	.010	.573	.982
2.0	.00	.968	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.954	.982	1.00	1.00	.996	.988	.972	.917	.995	.995	.978	1.00	.999	.999	.996	.991	.969	.997	.988
2.0	.50	.989	.999	.998	.996	.991	.982	.924	.999	.998	.990	.995	.995	.992	.978	.956	.857	.997	.998	.990	.997	.997	.993	.981	.966	.877	.997	1.00
2.0	.75	.991	.991	.986	.982	.956	.911	.698	.984	1.00	.992	.994	.989	.977	.946	.897	.697	.990	1.00	.993	.996	.993	.988	.967	.911	.683	.992	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=4 N=9 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.216	.348	.264	.180	.106	.051	.008	.109	.341	.278	.360	.270	.190	.090	.036	.003	.206	.912	.250	.373	.307	.221	.115	.050	.008	.167	.716
0.5	.50	.217	.368	.277	.200	.115	.067	.016	.216	.818	.280	.402	.296	.196	.092	.053	.017	.319	.968	.268	.374	.297	.192	.088	.040	.010	.246	.907
0.5	.85	.253	.408	.302	.200	.094	.042	.008	.502	.989	.247	.383	.282	.186	.089	.046	.013	.497	.984	.247	.404	.313	.204	.095	.046	.008	.529	.988
2.0	.00	.964	1.00	1.00	1.00	1.00	.999	.991	1.00	.958	.963	.987	.979	.970	.951	.909	.753	.973	.993	.970	.999	.997	.994	.986	.965	.895	.989	.981
2.0	.50	.967	1.00	.997	.995	.979	.962	.871	.997	.994	.974	.987	.979	.967	.941	.891	.717	.977	1.00	.971	.989	.985	.979	.962	.925	.768	.985	.998
2.0	.85	.995	.977	.956	.930	.851	.746	.443	.885	.998	.992	.967	.948	.914	.841	.743	.447	.874	.998	.991	.971	.954	.931	.869	.760	.447	.891	.995

C=4 N=9 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.236	.349	.263	.168	.096	.048	.008	.100	.426	.355	.360	.287	.208	.097	.056	.009	.274	.963	.301	.348	.274	.186	.094	.047	.004	.146	.776
0.5	.50	.268	.360	.273	.183	.098	.045	.008	.196	.851	.364	.365	.269	.178	.088	.040	.004	.301	.988	.342	.366	.295	.207	.107	.046	.008	.254	.947
0.5	.85	.380	.384	.305	.214	.110	.066	.013	.432	.989	.415	.376	.286	.177	.092	.039	.009	.406	.979	.416	.401	.316	.211	.085	.041	.012	.428	.972
2.0	.00	.957	1.00	1.00	1.00	.999	.998	.960	.999	.962	.963	.981	.966	.944	.889	.827	.561	.948	.999	.957	.993	.991	.982	.956	.921	.769	.964	.989
2.0	.50	.966	.996	.993	.984	.964	.926	.781	.992	.993	.962	.961	.952	.932	.869	.792	.551	.953	.997	.962	.980	.970	.955	.925	.866	.636	.964	.999
2.0	.85	.981	.954	.935	.905	.825	.725	.417	.879	1.00	.975	.954	.938	.901	.806	.698	.382	.868	.997	.965	.935	.918	.886	.796	.684	.379	.858	.998

C=4 N=9 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.253	.321	.266	.205	.111	.051	.012	.131	.471	.431	.366	.294	.209	.113	.048	.011	.281	.979	.329	.335	.265	.190	.095	.044	.007	.158	.825
0.5	.50	.302	.360	.270	.181	.102	.044	.010	.194	.888	.436	.385	.302	.218	.116	.064	.011	.310	.982	.371	.377	.289	.192	.105	.048	.005	.253	.953
0.5	.90	.487	.394	.304	.198	.092	.044	.004	.308	.947	.498	.372	.280	.179	.091	.040	.007	.309	.927	.527	.410	.305	.207	.112	.062	.009	.332	.943
2.0	.00	.930	1.00	1.00	.998	.989	.981	.917	.989	.951	.943	.946	.928	.905	.826	.734	.460	.914	1.00	.957	.986	.983	.969	.932	.884	.676	.943	.987
2.0	.50	.964	.992	.987	.978	.944	.909	.731	.983	.992	.933	.934	.912	.879	.797	.703	.411	.903	.999	.945	.960	.941	.921	.877	.805	.521	.938	1.00
2.0	.90	.967	.916	.888	.836	.717	.584	.282	.689	.975	.972	.919	.878	.836	.712	.554	.242	.684	.987	.963	.899	.873	.804	.680	.547	.254	.656	.975

C=4 N=9 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.287	.344	.266	.196	.104	.048	.006	.103	.557	.476	.374	.298	.207	.103	.047	.008	.267	.969	.362	.337	.268	.187	.086	.038	.009	.165	.889
0.5	.50	.274	.311	.240	.166	.083	.042	.004	.163	.881	.484	.378	.310	.222	.109	.051	.008	.276	.972	.400	.355	.278	.205	.109	.050	.009	.237	.962
0.5	.90	.510	.377	.301	.212	.113	.058	.007	.309	.930	.578	.406	.307	.202	.105	.044	.007	.292	.925	.538	.390	.298	.210	.112	.056	.003	.276	.934
2.0	.00	.958	.998	.998	.997	.991	.971	.897	.991	.964	.925	.901	.879	.834	.745	.620	.332	.839	.996	.937	.978	.973	.959	.912	.837	.584	.934	.986
2.0	.50	.938	.982	.972	.958	.922	.884	.664	.970	.993	.920	.893	.873	.838	.744	.614	.326	.842	.998	.927	.938	.919	.885	.832	.742	.474	.906	1.00
2.0	.90	.960	.894	.872	.813	.702	.553	.239	.685	.979	.936	.865	.839	.788	.674	.541	.236	.682	.972	.937	.876	.845	.788	.681	.531	.244	.671	.970

C=4 N=12 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.118	.381	.300	.209	.107	.055	.014	.108	.030	.087	.412	.311	.192	.107	.055	.013	.134	.231	.088	.397	.308	.212	.115	.066	.013	.132	.129
0.5	.50	.066	.404	.295	.186	.092	.049	.016	.302	.586	.062	.406	.300	.201	.107	.053	.012	.343	.669	.048	.392	.296	.203	.113	.062	.018	.326	.672
2.0	.00	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.974	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.995	.998	1.00	1.00	1.00	1.00	1.00	.999	1.00	.987
2.0	.50	1.00	1.00	1.00	1.00	1.00	.999	.994	1.00	.999	1.00	1.00	1.00	1.00	1.00	.999	.992	1.00	.998	.999	1.00	1.00	1.00	1.00	.999	.990	1.00	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=4 N=12 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.185	.342	.266	.185	.083	.050	.010	.092	.095	.248	.401	.320	.202	.101	.055	.016	.199	.660	.228	.385	.287	.201	.108	.052	.006	.143	.396
0.5	.50	.214	.374	.306	.218	.126	.059	.014	.303	.692	.210	.402	.314	.208	.108	.051	.015	.358	.879	.214	.407	.294	.188	.094	.049	.009	.321	.852
0.5	.75	.172	.422	.319	.219	.116	.055	.016	.739	.988	.136	.375	.286	.189	.102	.055	.016	.699	.991	.160	.437	.326	.213	.102	.048	.013	.739	.987
2.0	.00	.992	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.964	.998	1.00	1.00	1.00	.999	.999	.978	1.00	.999	.998	1.00	1.00	1.00	1.00	.998	.992	1.00	.990
2.0	.50	.994	1.00	1.00	1.00	.999	.997	.983	1.00	.996	.992	1.00	1.00	1.00	.994	.982	.926	1.00	1.00	.996	1.00	1.00	.998	.997	.990	.957	1.00	.998
2.0	.75	.999	.999	.997	.994	.987	.971	.865	.995	1.00	.998	.999	.998	.996	.989	.976	.875	.997	1.00	.999	.996	.995	.994	.984	.967	.871	.994	1.00

C=4 N=12 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.250	.368	.269	.193	.109	.057	.009	.112	.184	.354	.372	.277	.184	.084	.036	.007	.252	.911	.318	.361	.275	.195	.093	.050	.012	.143	.598
0.5	.50	.332	.389	.299	.203	.111	.063	.014	.245	.764	.346	.368	.280	.186	.097	.056	.012	.367	.968	.353	.385	.296	.212	.114	.056	.009	.324	.921
0.5	.85	.309	.380	.286	.180	.102	.053	.016	.579	.997	.333	.385	.288	.211	.105	.046	.011	.577	.991	.320	.408	.308	.202	.088	.045	.007	.566	.996
2.0	.00	.989	1.00	1.00	1.00	1.00	1.00	.999	1.00	.962	.992	.998	.996	.994	.982	.959	.878	.993	1.00	.992	1.00	1.00	1.00	.998	.994	.971	1.00	.992
2.0	.50	.992	1.00	1.00	.999	.995	.992	.963	.999	.995	.991	.996	.992	.984	.969	.954	.860	.994	1.00	.993	.998	.997	.994	.980	.965	.878	.996	1.00
2.0	.85	.999	.989	.978	.960	.918	.860	.631	.930	.997	1.00	.987	.977	.960	.909	.855	.607	.917	.998	.999	.989	.983	.963	.926	.871	.656	.936	.998

C=4 N=12 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.290	.322	.257	.191	.089	.041	.008	.101	.261	.457	.392	.304	.207	.109	.049	.009	.306	.964	.373	.358	.284	.197	.112	.050	.006	.181	.735
0.5	.50	.358	.370	.294	.194	.106	.047	.010	.242	.821	.470	.399	.308	.217	.099	.042	.010	.377	.990	.441	.367	.276	.188	.099	.056	.012	.292	.960
0.5	.85	.487	.404	.300	.218	.123	.060	.011	.506	.987	.504	.383	.294	.196	.093	.045	.010	.465	.981	.491	.420	.314	.219	.116	.051	.007	.494	.990
2.0	.00	.984	1.00	1.00	1.00	1.00	.999	.991	1.00	.961	.989	.983	.980	.976	.949	.897	.744	.979	1.00	.984	.998	.998	.996	.986	.974	.897	.994	.992
2.0	.50	.989	.999	.999	.997	.992	.987	.922	1.00	.995	.984	.981	.977	.967	.935	.877	.683	.978	1.00	.985	.995	.990	.980	.960	.920	.786	.995	1.00
2.0	.85	.991	.975	.964	.938	.892	.823	.586	.923	.999	.987	.972	.963	.935	.883	.813	.557	.906	.995	.993	.977	.966	.938	.881	.806	.561	.905	.998

C=4 N=12 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.311	.325	.253	.183	.092	.053	.010	.095	.323	.520	.363	.276	.187	.093	.039	.008	.310	.983	.431	.341	.267	.194	.102	.054	.010	.169	.809
0.5	.50	.398	.365	.285	.197	.094	.046	.006	.231	.849	.525	.373	.280	.198	.108	.047	.005	.325	.979	.486	.374	.308	.214	.112	.051	.010	.301	.966
0.5	.90	.597	.399	.309	.191	.094	.048	.007	.359	.954	.651	.401	.302	.203	.094	.045	.007	.327	.944	.619	.400	.316	.205	.088	.041	.007	.369	.955
2.0	.00	.977	1.00	1.00	1.00	1.00	.997	.978	1.00	.959	.984	.975	.966	.948	.908	.838	.596	.961	1.00	.975	.997	.993	.990	.972	.953	.833	.985	.986
2.0	.50	.985	.998	.997	.990	.979	.964	.869	.996	.997	.985	.974	.962	.939	.882	.818	.588	.952	.999	.978	.984	.974	.964	.936	.888	.698	.977	1.00
2.0	.90	.986	.955	.939	.906	.818	.722	.429	.791	.986	.981	.942	.920	.876	.791	.695	.372	.759	.974	.988	.959	.931	.889	.805	.692	.410	.766	.988

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=4 N=12 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.339	.321	.258	.190	.099	.050	.003	.102	.376	.536	.353	.284	.204	.094	.046	.008	.287	.978	.466	.365	.288	.201	.103	.046	.007	.190	.838
0.5	.50	.398	.331	.252	.173	.096	.046	.005	.203	.852	.555	.378	.299	.198	.088	.049	.010	.297	.985	.498	.369	.290	.194	.096	.052	.007	.270	.967
0.5	.90	.626	.397	.310	.212	.115	.057	.010	.321	.941	.644	.393	.292	.196	.094	.046	.006	.275	.924	.681	.399	.306	.213	.125	.045	.008	.280	.937
2.0	.00	.978	1.00	.999	.999	.998	.991	.959	.999	.949	.967	.948	.937	.909	.850	.770	.492	.924	1.00	.973	.991	.982	.973	.940	.907	.731	.959	.992
2.0	.50	.979	.996	.996	.989	.975	.948	.837	.996	.996	.975	.948	.930	.896	.832	.746	.468	.911	.999	.968	.971	.958	.935	.892	.811	.587	.956	1.00
2.0	.90	.978	.926	.892	.850	.770	.654	.364	.740	.981	.972	.930	.893	.844	.740	.629	.361	.708	.977	.969	.911	.883	.845	.735	.644	.321	.706	.973

C=4 N=16 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.152	.406	.317	.214	.126	.061	.020	.129	.005	.112	.372	.288	.199	.099	.051	.013	.126	.106	.126	.417	.315	.222	.119	.065	.014	.138	.036
0.5	.50	.096	.383	.287	.207	.105	.053	.015	.397	.644	.073	.415	.327	.217	.116	.066	.014	.430	.672	.049	.389	.283	.193	.102	.051	.012	.415	.699
2.0	.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.964	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.994	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.995
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.998	1.00	1.00	1.00	1.00	1.00	1.00	.999	1.00	.999	.999	1.00	1.00	1.00	1.00	1.00	.998	1.00	1.00

C=4 N=16 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.246	.370	.269	.190	.098	.051	.012	.101	.025	.285	.382	.288	.200	.110	.059	.016	.251	.602	.285	.378	.303	.210	.101	.056	.011	.150	.252
0.5	.50	.247	.392	.310	.210	.112	.056	.014	.340	.664	.272	.398	.306	.213	.115	.058	.012	.438	.876	.278	.369	.278	.199	.100	.052	.011	.400	.867
0.5	.75	.204	.400	.305	.202	.091	.053	.012	.851	.998	.207	.402	.296	.205	.099	.051	.017	.832	.999	.196	.387	.298	.197	.101	.048	.015	.843	1.00
2.0	.00	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.969	1.00	1.00	1.00	1.00	1.00	1.00	.995	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.994
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	.996	1.00	.998	.998	1.00	1.00	1.00	1.00	.998	.988	1.00	1.00	.999	1.00	.999	.999	.999	.998	.985	1.00	.999
2.0	.75	1.00	1.00	.999	.998	.996	.990	.964	.999	1.00	1.00	.999	.999	.998	.996	.989	.952	.999	1.00	1.00	.999	.998	.995	.990	.984	.941	.998	1.00

C=4 N=16 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.313	.350	.272	.193	.100	.051	.007	.104	.080	.465	.387	.293	.202	.102	.055	.010	.310	.893	.411	.387	.293	.211	.104	.048	.009	.159	.477
0.5	.50	.401	.400	.309	.212	.100	.051	.008	.319	.778	.464	.393	.293	.187	.089	.044	.004	.466	.975	.463	.408	.311	.196	.105	.052	.009	.403	.920
0.5	.85	.436	.408	.306	.213	.112	.058	.012	.660	.997	.410	.404	.316	.213	.107	.054	.017	.665	.999	.413	.383	.287	.204	.102	.052	.009	.615	.995
2.0	.00	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.961	.997	1.00	1.00	1.00	.999	.993	.957	1.00	1.00	.998	1.00	1.00	1.00	1.00	.999	.991	1.00	.995
2.0	.50	1.00	1.00	1.00	1.00	.999	.997	.985	1.00	.999	.998	.999	.998	.997	.987	.981	.944	1.00	1.00	.998	1.00	.998	.998	.993	.991	.959	1.00	.999
2.0	.85	1.00	.998	.996	.993	.969	.940	.807	.968	1.00	1.00	.994	.990	.985	.972	.938	.794	.971	1.00	1.00	.998	.994	.990	.976	.941	.797	.972	1.00

C=4 N=16 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.342	.344	.288	.206	.103	.052	.007	.112	.161	.576	.396	.305	.199	.107	.049	.004	.377	.974	.497	.360	.273	.175	.088	.048	.011	.160	.660
0.5	.50	.463	.381	.287	.203	.110	.054	.014	.279	.809	.575	.372	.289	.202	.109	.052	.010	.420	.989	.538	.393	.306	.202	.098	.045	.004	.376	.959
0.5	.85	.604	.434	.322	.213	.115	.059	.010	.613	.992	.602	.402	.310	.212	.108	.052	.008	.540	.991	.600	.409	.302	.198	.114	.055	.011	.532	.989
2.0	.00	.993	1.00	1.00	1.00	1.00	1.00	.999	1.00	.962	.995	.996	.991	.988	.972	.949	.866	.995	1.00	.996	1.00	.999	.999	.999	.993	.970	.998	.995
2.0	.50	.999	1.00	.999	.999	.997	.996	.978	1.00	.999	.997	.997	.996	.993	.979	.953	.854	.997	1.00	.998	.998	.998	.994	.983	.970	.906	.999	1.00
2.0	.85	1.00	.993	.988	.977	.951	.906	.749	.958	.999	1.00	.988	.984	.965	.934	.889	.727	.954	.999	1.00	.991	.984	.971	.932	.881	.716	.946	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=4 N=16 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.392	.324	.249	.173	.088	.040	.015	.097	.195	.617	.399	.301	.189	.080	.042	.009	.374	.990	.514	.356	.286	.192	.092	.049	.010	.173	.725
0.5	.50	.452	.355	.272	.189	.091	.047	.010	.261	.831	.663	.396	.298	.214	.094	.040	.009	.410	.988	.570	.381	.283	.191	.101	.047	.005	.339	.963
0.5	.90	.709	.409	.319	.210	.106	.046	.006	.396	.965	.745	.428	.323	.229	.117	.063	.013	.401	.967	.749	.420	.315	.223	.113	.055	.009	.374	.962
2.0	.00	.993	1.00	1.00	1.00	1.00	1.00	.993	1.00	.961	.994	.990	.982	.970	.949	.901	.741	.985	1.00	.998	.999	.999	.998	.994	.982	.939	.996	.995
2.0	.50	.997	.999	.999	.998	.992	.991	.961	.999	.999	.992	.986	.981	.963	.946	.903	.722	.983	1.00	.993	.995	.992	.987	.966	.947	.834	.996	1.00
2.0	.90	.998	.972	.961	.937	.873	.799	.569	.832	.993	.997	.975	.957	.930	.870	.790	.566	.811	.993	1.00	.978	.969	.941	.889	.809	.559	.831	.993

C=4 N=16 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.437	.321	.251	.181	.094	.040	.008	.106	.245	.673	.368	.293	.200	.111	.060	.014	.331	.988	.516	.318	.243	.176	.092	.044	.006	.170	.778
0.5	.50	.489	.326	.230	.173	.092	.039	.008	.221	.859	.677	.364	.279	.198	.103	.047	.010	.329	.979	.593	.372	.295	.203	.116	.066	.010	.316	.975
0.5	.90	.700	.381	.299	.206	.108	.045	.012	.337	.947	.786	.395	.304	.207	.114	.055	.005	.338	.935	.786	.408	.325	.219	.122	.054	.012	.326	.941
2.0	.00	.992	1.00	1.00	1.00	1.00	.998	.988	1.00	.962	.991	.974	.965	.942	.913	.857	.606	.962	1.00	.992	.998	.997	.992	.985	.961	.862	.988	.995
2.0	.50	.996	.999	.998	.994	.990	.973	.918	.999	1.00	.996	.979	.972	.957	.908	.838	.619	.960	1.00	.995	.993	.988	.978	.956	.925	.752	.991	1.00
2.0	.90	.992	.954	.938	.911	.841	.761	.506	.805	.982	.991	.954	.929	.892	.820	.715	.459	.758	.986	.992	.944	.927	.892	.823	.725	.440	.778	.980

C=6 N=4 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.028	.361	.278	.190	.097	.059	.024	.089	.572	.012	.368	.280	.196	.110	.074	.035	.109	.719	.013	.385	.310	.224	.127	.073	.040	.123	.697
0.5	.50	.004	.379	.296	.198	.116	.076	.039	.120	.738	.003	.364	.283	.204	.124	.089	.044	.140	.765	.003	.414	.317	.196	.098	.066	.033	.123	.788
2.0	.00	.861	1.00	1.00	1.00	1.00	1.00	.958	1.00	.975	.889	1.00	1.00	.998	.998	.981	.823	.997	.982	.879	1.00	1.00	.999	.997	.979	.872	.996	.985
2.0	.50	.890	.999	.999	.993	.976	.922	.783	.997	.994	.893	.998	.995	.988	.969	.926	.729	.991	.986	.895	.995	.995	.990	.974	.912	.704	.988	.987

C=6 N=4 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.033	.314	.237	.140	.075	.037	.012	.074	.688	.035	.377	.284	.198	.113	.072	.028	.134	.881	.049	.358	.275	.178	.091	.051	.025	.100	.831
0.5	.50	.045	.370	.280	.186	.099	.071	.029	.127	.828	.031	.375	.289	.205	.123	.082	.039	.161	.870	.033	.389	.289	.215	.113	.066	.033	.140	.862
0.5	.75	.032	.396	.314	.213	.129	.086	.044	.278	.898	.022	.407	.311	.223	.132	.082	.043	.267	.907	.014	.373	.278	.184	.109	.078	.036	.261	.911
2.0	.00	.819	1.00	1.00	1.00	1.00	.995	.884	.999	.952	.870	.997	.995	.989	.956	.878	.605	.971	.992	.836	.998	.992	.988	.978	.923	.705	.977	.977
2.0	.50	.839	.998	.992	.986	.945	.884	.658	.973	.988	.859	.988	.983	.966	.915	.814	.535	.960	.992	.853	.990	.985	.969	.917	.845	.582	.963	.991
2.0	.75	.892	.982	.964	.919	.815	.682	.444	.968	.997	.892	.966	.957	.934	.826	.679	.445	.960	.995	.895	.980	.971	.933	.844	.670	.434	.971	.994

C=6 N=4 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.065	.321	.238	.172	.086	.050	.012	.087	.746	.086	.383	.282	.179	.092	.051	.022	.141	.920	.099	.348	.280	.195	.099	.045	.023	.131	.853
0.5	.50	.070	.356	.284	.187	.099	.053	.025	.116	.858	.079	.378	.277	.210	.115	.060	.022	.185	.936	.087	.382	.297	.190	.085	.051	.022	.144	.921
0.5	.85	.067	.410	.315	.209	.135	.099	.059	.419	.934	.048	.394	.302	.215	.129	.088	.043	.404	.932	.064	.410	.292	.188	.116	.090	.060	.433	.945
2.0	.00	.786	1.00	1.00	1.00	.994	.973	.796	.995	.965	.832	.974	.962	.931	.863	.740	.435	.909	.995	.829	.989	.986	.975	.945	.884	.573	.951	.983
2.0	.50	.832	.991	.985	.973	.923	.844	.572	.961	.984	.836	.965	.957	.919	.830	.693	.384	.906	.997	.833	.967	.961	.933	.860	.739	.446	.919	.993
2.0	.85	.913	.935	.897	.843	.661	.492	.233	.854	.989	.918	.935	.908	.856	.678	.509	.257	.856	.980	.906	.931	.897	.843	.667	.483	.228	.850	.979

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=6 N=4 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.081	.307	.244	.169	.090	.041	.011	.097	.766	.124	.346	.259	.160	.074	.038	.013	.144	.970	.099	.318	.241	.172	.075	.037	.008	.117	.879
0.5	.50	.113	.371	.301	.210	.111	.051	.016	.137	.893	.145	.385	.290	.195	.097	.057	.022	.206	.967	.131	.375	.295	.184	.102	.054	.019	.167	.941
0.5	.85	.126	.366	.277	.189	.090	.052	.023	.333	.955	.125	.373	.290	.185	.096	.052	.030	.358	.955	.123	.388	.283	.190	.089	.059	.023	.346	.970
2.0	.00	.766	.997	.994	.991	.972	.936	.726	.979	.958	.827	.942	.923	.879	.779	.629	.272	.862	.992	.784	.977	.964	.941	.889	.788	.452	.918	.980
2.0	.50	.788	.977	.964	.947	.874	.777	.471	.933	.988	.831	.928	.908	.861	.759	.599	.279	.860	.998	.793	.939	.913	.888	.789	.674	.361	.873	.987
2.0	.85	.847	.894	.857	.815	.658	.445	.190	.843	.981	.860	.912	.882	.810	.654	.440	.184	.850	.982	.849	.893	.853	.797	.643	.462	.201	.825	.988

C=6 N=4 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.109	.303	.241	.177	.084	.034	.008	.098	.787	.159	.332	.269	.168	.074	.033	.014	.180	.971	.144	.360	.281	.202	.120	.053	.009	.147	.913
0.5	.50	.120	.322	.245	.166	.097	.046	.013	.125	.905	.163	.336	.266	.175	.076	.037	.006	.183	.969	.153	.353	.275	.184	.084	.047	.012	.165	.961
0.5	.90	.187	.397	.293	.199	.093	.047	.022	.392	.912	.179	.402	.276	.175	.063	.029	.013	.376	.923	.172	.367	.279	.171	.065	.037	.016	.376	.923
2.0	.00	.761	.996	.992	.981	.957	.896	.626	.961	.963	.780	.883	.850	.796	.676	.524	.199	.775	.997	.739	.956	.941	.905	.815	.711	.365	.846	.978
2.0	.50	.799	.975	.963	.939	.865	.746	.445	.913	.990	.801	.893	.861	.812	.674	.479	.180	.825	.997	.794	.903	.887	.844	.744	.590	.275	.828	.990
2.0	.90	.855	.858	.827	.738	.550	.365	.143	.692	.925	.834	.840	.808	.736	.569	.356	.122	.713	.916	.832	.840	.799	.736	.524	.338	.089	.689	.923

C=6 N=4 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.104	.296	.232	.165	.093	.041	.012	.107	.809	.212	.337	.277	.179	.087	.046	.010	.209	.970	.148	.331	.250	.184	.104	.044	.011	.144	.913
0.5	.50	.118	.278	.222	.149	.091	.048	.012	.124	.892	.227	.365	.286	.201	.093	.042	.009	.234	.974	.187	.366	.270	.177	.092	.041	.014	.186	.963
0.5	.90	.226	.361	.282	.179	.076	.031	.014	.337	.923	.248	.383	.273	.174	.079	.037	.012	.324	.909	.243	.383	.296	.189	.074	.034	.015	.340	.914
2.0	.00	.763	.991	.988	.973	.935	.864	.588	.938	.971	.761	.839	.806	.758	.642	.453	.150	.760	.996	.751	.936	.914	.874	.771	.639	.300	.820	.977
2.0	.50	.745	.956	.941	.901	.819	.681	.357	.870	.988	.731	.817	.775	.714	.572	.388	.129	.721	.992	.761	.895	.864	.818	.699	.543	.222	.800	.990
2.0	.90	.802	.823	.778	.698	.532	.362	.124	.683	.927	.767	.778	.744	.675	.499	.302	.069	.669	.911	.768	.791	.746	.680	.518	.323	.082	.675	.927

C=6 N=6 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.025	.354	.267	.180	.089	.045	.015	.091	.218	.016	.392	.301	.208	.112	.056	.023	.115	.408	.021	.387	.294	.190	.095	.053	.017	.098	.352
0.5	.50	.014	.402	.309	.212	.119	.062	.034	.151	.457	.008	.392	.291	.200	.118	.079	.028	.152	.542	.005	.397	.305	.219	.116	.071	.023	.140	.547
2.0	.00	.924	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.954	.962	1.00	1.00	1.00	1.00	.998	.976	1.00	.985	.960	1.00	1.00	1.00	1.00	.999	.989	1.00	.982
2.0	.50	.965	1.00	.999	.999	.996	.991	.928	1.00	.996	.963	1.00	.998	.997	.996	.986	.905	.998	.996	.958	.999	.999	.998	.994	.988	.903	.998	.992

C=6 N=6 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.065	.342	.265	.184	.091	.048	.015	.093	.346	.067	.392	.297	.212	.111	.055	.022	.138	.720	.075	.397	.305	.206	.102	.054	.016	.110	.581
0.5	.50	.057	.356	.266	.182	.094	.052	.013	.125	.626	.055	.409	.308	.200	.107	.055	.016	.166	.768	.062	.374	.294	.202	.097	.053	.014	.157	.770
0.5	.75	.035	.387	.302	.198	.105	.062	.023	.359	.857	.033	.378	.285	.214	.110	.067	.026	.379	.848	.026	.367	.289	.206	.111	.071	.030	.342	.864
2.0	.00	.934	1.00	1.00	1.00	1.00	.999	.990	1.00	.968	.945	1.00	.997	.995	.990	.971	.853	.991	.987	.940	1.00	1.00	.999	.997	.993	.916	.998	.979
2.0	.50	.956	.998	.998	.998	.994	.981	.861	.999	.992	.958	.998	.996	.993	.978	.945	.792	.990	.995	.956	.997	.995	.993	.980	.953	.792	.990	.997
2.0	.75	.965	.995	.989	.974	.952	.897	.650	.995	1.00	.972	.994	.993	.979	.947	.881	.652	.993	.997	.963	.993	.985	.977	.940	.872	.618	.991	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=6 N=6 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.114	.371	.299	.200	.103	.056	.011	.111	.468	.115	.372	.286	.200	.106	.052	.017	.167	.848	.128	.352	.268	.193	.102	.052	.015	.119	.715
0.5	.50	.109	.334	.235	.171	.079	.037	.009	.119	.702	.142	.366	.296	.208	.102	.053	.018	.213	.919	.127	.366	.269	.199	.099	.048	.019	.177	.843
0.5	.85	.091	.394	.298	.190	.101	.056	.027	.526	.965	.084	.390	.284	.186	.100	.061	.027	.524	.954	.085	.418	.324	.227	.113	.065	.026	.529	.957
2.0	.00	.909	1.00	1.00	1.00	1.00	.997	.964	1.00	.956	.919	.989	.985	.976	.942	.901	.684	.965	.993	.914	.997	.994	.990	.980	.959	.828	.982	.981
2.0	.50	.919	.998	.998	.998	.986	.966	.842	.992	.982	.936	.991	.984	.972	.933	.866	.630	.974	.998	.935	.993	.991	.978	.952	.915	.700	.981	.993
2.0	.85	.963	.966	.948	.920	.828	.701	.378	.933	.993	.974	.975	.956	.920	.841	.728	.378	.938	.998	.970	.963	.943	.915	.831	.718	.366	.929	.996

C=6 N=6 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.116	.327	.256	.172	.092	.051	.008	.108	.532	.187	.365	.285	.195	.088	.041	.011	.202	.944	.198	.373	.292	.205	.106	.047	.006	.138	.798
0.5	.50	.145	.351	.275	.188	.097	.047	.009	.136	.777	.195	.395	.314	.204	.101	.050	.009	.232	.952	.192	.368	.283	.190	.094	.045	.011	.186	.925
0.5	.85	.174	.378	.300	.204	.094	.052	.017	.424	.979	.180	.364	.287	.188	.090	.052	.015	.441	.985	.186	.410	.313	.198	.089	.038	.013	.469	.988
2.0	.00	.890	1.00	.999	.999	.996	.992	.933	.996	.957	.918	.968	.960	.933	.881	.807	.513	.924	.996	.911	.990	.985	.981	.957	.919	.699	.965	.987
2.0	.50	.909	1.00	.997	.988	.970	.931	.744	.983	.983	.909	.965	.948	.925	.859	.774	.479	.937	1.00	.918	.990	.982	.968	.923	.857	.579	.970	.994
2.0	.85	.938	.954	.933	.889	.794	.679	.346	.916	.995	.936	.942	.925	.883	.790	.660	.322	.902	.993	.937	.944	.924	.895	.810	.670	.326	.916	.999

C=6 N=6 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.138	.319	.255	.185	.101	.045	.009	.107	.573	.226	.353	.262	.162	.077	.037	.007	.200	.965	.214	.367	.294	.206	.102	.045	.008	.143	.841
0.5	.50	.169	.323	.259	.180	.095	.049	.007	.137	.798	.250	.362	.284	.201	.099	.039	.007	.259	.964	.244	.355	.289	.199	.110	.048	.008	.203	.923
0.5	.90	.261	.375	.297	.200	.100	.051	.011	.416	.977	.270	.401	.303	.200	.088	.039	.011	.424	.985	.278	.422	.330	.204	.100	.052	.014	.449	.972
2.0	.00	.888	.999	.998	.997	.995	.991	.889	.995	.964	.886	.938	.922	.896	.801	.700	.374	.886	.997	.886	.979	.974	.957	.911	.858	.604	.927	.980
2.0	.50	.897	.991	.988	.976	.949	.902	.690	.972	.982	.907	.951	.932	.896	.809	.692	.367	.911	.996	.874	.960	.941	.916	.864	.778	.486	.920	.994
2.0	.90	.944	.917	.887	.832	.708	.549	.197	.819	.982	.954	.923	.894	.837	.700	.533	.187	.827	.989	.940	.916	.886	.832	.710	.563	.192	.817	.982

C=6 N=6 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.157	.300	.235	.175	.096	.053	.006	.103	.594	.310	.380	.285	.202	.089	.040	.003	.253	.980	.216	.361	.280	.186	.085	.034	.005	.133	.877
0.5	.50	.192	.316	.249	.177	.105	.055	.008	.143	.835	.294	.377	.306	.204	.097	.043	.008	.270	.985	.221	.322	.250	.171	.076	.033	.006	.181	.944
0.5	.90	.310	.382	.289	.193	.099	.057	.012	.390	.979	.338	.370	.289	.193	.084	.042	.008	.340	.969	.342	.388	.288	.184	.067	.027	.006	.359	.969
2.0	.00	.883	.998	.998	.996	.990	.971	.837	.991	.954	.871	.915	.891	.857	.753	.621	.298	.866	.998	.856	.972	.961	.942	.886	.808	.516	.912	.979
2.0	.50	.866	.980	.969	.948	.906	.848	.582	.940	.987	.881	.901	.876	.830	.731	.591	.245	.851	.999	.877	.953	.936	.902	.834	.734	.405	.907	.993
2.0	.90	.906	.878	.857	.789	.671	.518	.183	.780	.979	.892	.872	.835	.783	.664	.500	.176	.771	.971	.904	.883	.854	.802	.671	.502	.180	.768	.983

C=6 N=9 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.047	.383	.295	.203	.112	.066	.010	.115	.036	.010	.402	.298	.201	.109	.062	.017	.117	.149	.026	.387	.292	.195	.095	.046	.013	.098	.111
0.5	.50	.016	.399	.299	.194	.105	.054	.012	.153	.282	.006	.388	.296	.194	.102	.048	.015	.178	.363	.007	.376	.310	.222	.114	.062	.012	.170	.381
2.0	.00	.980	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.963	.995	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.993	.987	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.976
2.0	.50	.994	1.00	1.00	1.00	1.00	1.00	.995	1.00	.992	.989	1.00	1.00	1.00	1.00	1.00	.997	1.00	.994	.996	1.00	1.00	1.00	1.00	1.00	.992	1.00	.997

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further.

C=6 N=9 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.119	.382	.297	.210	.107	.061	.010	.108	.140	.088	.368	.276	.196	.110	.067	.017	.147	.534	.077	.363	.267	.173	.090	.048	.009	.097	.323
0.5	.50	.088	.395	.299	.198	.097	.060	.013	.157	.497	.065	.386	.295	.196	.100	.056	.011	.198	.657	.076	.397	.305	.185	.094	.050	.010	.201	.656
0.5	.75	.057	.408	.316	.218	.117	.063	.012	.529	.852	.049	.391	.286	.182	.097	.050	.014	.497	.843	.042	.367	.274	.182	.097	.055	.021	.538	.887
2.0	.00	.980	1.00	1.00	1.00	1.00	1.00	.999	1.00	.973	.988	1.00	1.00	1.00	1.00	.999	.984	1.00	.996	.982	1.00	1.00	1.00	1.00	.999	.997	1.00	.987
2.0	.50	.987	1.00	1.00	1.00	1.00	.999	.983	1.00	.988	.986	1.00	.999	.999	.993	.989	.949	1.00	.997	.987	1.00	1.00	1.00	.998	.996	.969	1.00	.994
2.0	.75	.991	.998	.996	.993	.987	.971	.873	1.00	.999	.993	.996	.996	.996	.992	.977	.876	.997	.999	.998	.998	.996	.994	.987	.972	.871	1.00	1.00

C=6 N=9 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.136	.351	.272	.180	.097	.050	.014	.107	.225	.189	.391	.287	.199	.093	.045	.008	.187	.820	.180	.351	.281	.184	.086	.047	.006	.110	.543
0.5	.50	.146	.362	.284	.195	.110	.065	.011	.167	.605	.179	.392	.316	.216	.111	.052	.009	.273	.882	.176	.375	.291	.199	.104	.057	.012	.201	.810
0.5	.85	.114	.363	.290	.199	.099	.055	.016	.658	.992	.136	.368	.292	.189	.098	.054	.009	.660	.986	.133	.402	.304	.208	.084	.050	.011	.670	.988
2.0	.00	.977	1.00	1.00	1.00	1.00	1.00	.999	1.00	.969	.986	.997	.996	.995	.992	.983	.912	.994	.997	.974	1.00	1.00	1.00	1.00	.997	.958	1.00	.984
2.0	.50	.980	1.00	1.00	1.00	1.00	.996	.957	1.00	.994	.984	.998	.997	.992	.978	.955	.851	.995	.999	.985	1.00	.999	.995	.990	.981	.897	.997	1.00
2.0	.85	.994	.991	.985	.967	.937	.877	.631	.972	1.00	.992	.991	.987	.975	.943	.885	.669	.982	1.00	.995	.991	.985	.975	.942	.886	.648	.980	1.00

C=6 N=9 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.199	.346	.261	.188	.096	.049	.008	.111	.320	.286	.386	.294	.195	.112	.054	.008	.256	.933	.229	.368	.279	.180	.081	.043	.007	.116	.655
0.5	.50	.204	.366	.283	.203	.109	.051	.011	.171	.664	.278	.393	.303	.196	.109	.051	.009	.309	.955	.255	.376	.285	.176	.092	.050	.008	.206	.888
0.5	.85	.247	.394	.300	.199	.099	.045	.010	.583	.992	.266	.389	.314	.214	.103	.058	.007	.575	.996	.268	.409	.323	.214	.090	.049	.007	.562	.994
2.0	.00	.964	1.00	1.00	1.00	1.00	1.00	.994	1.00	.949	.972	.991	.987	.978	.962	.931	.787	.974	.995	.966	1.00	1.00	1.00	.996	.984	.921	.996	.985
2.0	.50	.978	1.00	1.00	.999	.996	.985	.929	1.00	.991	.973	.989	.984	.980	.956	.905	.741	.984	1.00	.978	.996	.994	.987	.966	.933	.813	.989	.999
2.0	.85	.988	.978	.969	.947	.907	.846	.611	.963	.999	.990	.984	.972	.958	.915	.840	.581	.963	.997	.986	.979	.968	.953	.907	.842	.588	.962	1.00

C=6 N=9 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.224	.368	.289	.202	.092	.046	.004	.099	.380	.369	.402	.305	.198	.112	.064	.018	.289	.966	.265	.337	.257	.174	.092	.049	.008	.131	.712
0.5	.50	.239	.354	.283	.191	.109	.054	.007	.180	.731	.342	.374	.288	.189	.091	.048	.006	.306	.977	.305	.372	.289	.202	.099	.051	.012	.233	.920
0.5	.90	.351	.394	.299	.203	.090	.035	.003	.509	.984	.376	.403	.306	.211	.105	.057	.011	.498	.987	.368	.420	.310	.208	.098	.049	.008	.497	.987
2.0	.00	.958	1.00	1.00	1.00	1.00	.999	.989	1.00	.959	.970	.986	.976	.958	.914	.852	.633	.967	.996	.963	.996	.995	.992	.982	.952	.841	.988	.993
2.0	.50	.958	.996	.992	.990	.985	.965	.889	.991	.989	.972	.980	.971	.954	.911	.838	.601	.970	.998	.967	.996	.991	.984	.960	.903	.719	.988	.998
2.0	.90	.985	.966	.951	.911	.827	.710	.402	.885	.996	.990	.973	.958	.925	.845	.743	.427	.894	.998	.984	.949	.924	.884	.798	.689	.387	.847	.996

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=6 N=9 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.217	.314	.241	.171	.082	.036	.007	.093	.393	.392	.367	.299	.207	.100	.044	.009	.302	.977	.295	.342	.264	.194	.101	.045	.005	.160	.763
0.5	.50	.267	.328	.249	.185	.088	.044	.005	.153	.758	.394	.350	.262	.184	.106	.050	.008	.310	.989	.338	.353	.270	.197	.108	.048	.006	.236	.938
0.5	.90	.430	.380	.297	.207	.113	.056	.013	.446	.987	.484	.420	.333	.222	.095	.036	.005	.449	.974	.459	.397	.296	.195	.091	.040	.011	.417	.982
2.0	.00	.960	1.00	1.00	.999	.997	.993	.969	.996	.965	.954	.962	.952	.929	.867	.772	.498	.942	.998	.956	.996	.990	.986	.973	.937	.780	.978	.981
2.0	.50	.963	.999	.998	.995	.980	.961	.844	.990	.993	.957	.955	.945	.927	.862	.767	.509	.946	.999	.956	.988	.981	.960	.922	.857	.638	.962	.998
2.0	.90	.963	.942	.916	.880	.795	.688	.394	.863	.996	.968	.947	.926	.880	.784	.646	.351	.851	.993	.965	.941	.920	.877	.779	.661	.343	.849	.993

C=6 N=12 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.070	.392	.305	.208	.102	.052	.014	.108	.008	.020	.369	.279	.177	.086	.042	.008	.104	.042	.030	.362	.294	.188	.098	.046	.010	.111	.030
0.5	.50	.029	.386	.297	.202	.103	.060	.012	.178	.228	.012	.404	.316	.204	.120	.064	.018	.193	.285	.007	.403	.299	.192	.104	.058	.017	.187	.299
2.0	.00	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.976	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.993	.995	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.986
2.0	.50	.998	1.00	1.00	1.00	1.00	1.00	.999	1.00	.995	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.998	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.997

C=6 N=12 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.132	.393	.313	.200	.113	.063	.008	.122	.045	.110	.377	.273	.188	.122	.060	.012	.171	.373	.128	.399	.302	.207	.093	.053	.017	.119	.167
0.5	.50	.124	.401	.313	.218	.123	.060	.011	.190	.388	.089	.378	.276	.195	.098	.052	.017	.241	.603	.093	.383	.294	.209	.101	.052	.014	.233	.573
0.5	.75	.071	.409	.322	.214	.102	.049	.010	.698	.920	.071	.402	.290	.196	.102	.051	.015	.692	.912	.061	.439	.330	.208	.115	.066	.017	.695	.912
2.0	.00	.992	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.963	.997	1.00	1.00	1.00	1.00	1.00	.998	1.00	.992	.993	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.985
2.0	.50	.998	1.00	1.00	1.00	1.00	1.00	.999	1.00	.996	1.00	1.00	1.00	1.00	1.00	1.00	.995	1.00	.997	.999	1.00	1.00	1.00	1.00	1.00	.996	1.00	.997
2.0	.75	1.00	1.00	1.00	1.00	.998	.995	.962	1.00	1.00	1.00	1.00	1.00	1.00	.999	.995	.970	1.00	1.00	.997	1.00	1.00	1.00	.997	.995	.959	1.00	1.00

C=6 N=12 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.199	.361	.284	.199	.110	.053	.012	.117	.098	.251	.395	.305	.222	.105	.054	.012	.243	.744	.210	.371	.289	.212	.104	.044	.011	.134	.358
0.5	.50	.222	.377	.279	.187	.112	.054	.013	.182	.502	.252	.419	.330	.222	.110	.068	.009	.331	.837	.258	.390	.303	.228	.122	.063	.016	.268	.756
0.5	.85	.163	.405	.307	.203	.097	.045	.012	.770	.998	.143	.400	.297	.187	.089	.045	.012	.789	.994	.155	.393	.301	.208	.095	.056	.014	.773	.995
2.0	.00	.989	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.958	.993	1.00	.999	.999	.997	.991	.962	.998	.997	.996	1.00	1.00	1.00	1.00	1.00	.996	1.00	.987
2.0	.50	.993	1.00	.999	.999	.999	.998	.990	.999	.995	1.00	.999	.999	.999	.997	.992	.960	.999	.999	.996	1.00	1.00	.999	.997	.993	.969	1.00	1.00
2.0	.85	.999	.995	.992	.986	.970	.944	.800	.988	.998	1.00	.993	.991	.985	.970	.940	.807	.984	1.00	1.00	.999	.998	.991	.980	.949	.815	.997	1.00

C=6 N=12 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.247	.360	.289	.200	.114	.056	.012	.121	.164	.351	.411	.311	.218	.110	.047	.014	.307	.894	.326	.385	.303	.190	.109	.051	.008	.144	.550
0.5	.50	.298	.362	.284	.191	.086	.052	.010	.178	.625	.318	.367	.289	.205	.105	.056	.009	.360	.945	.325	.368	.266	.183	.093	.050	.006	.254	.864
0.5	.85	.322	.401	.309	.208	.109	.054	.008	.657	.996	.332	.382	.279	.180	.096	.047	.011	.632	.999	.320	.388	.291	.199	.084	.043	.008	.647	.999
2.0	.00	.992	1.00	1.00	1.00	1.00	1.00	.999	1.00	.975	.991	1.00	.998	.993	.986	.972	.904	.999	.999	.992	1.00	1.00	.999	.998	.996	.981	.999	.989
2.0	.50	.989	.999	.998	.997	.997	.995	.984	.999	.991	.995	.999	.997	.994	.983	.966	.875	.996	1.00	.993	.997	.997	.996	.993	.986	.938	.996	.999
2.0	.85	.994	.992	.990	.987	.958	.925	.771	.983	.999	.999	.993	.985	.975	.949	.911	.761	.981	1.00	.997	.992	.984	.975	.941	.908	.760	.982	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further.

C=6 N=12 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.279	.327	.269	.189	.105	.049	.009	.113	.216	.421	.364	.271	.188	.095	.051	.011	.327	.967	.366	.359	.277	.202	.125	.071	.016	.172	.631
0.5	.50	.326	.352	.286	.204	.109	.061	.011	.186	.642	.439	.392	.300	.202	.105	.050	.007	.376	.981	.386	.369	.275	.193	.108	.051	.008	.270	.899
0.5	.90	.470	.408	.303	.204	.102	.051	.009	.559	.991	.458	.384	.302	.209	.103	.050	.009	.543	.990	.449	.384	.286	.196	.090	.049	.011	.502	.988
2.0	.00	.988	1.00	1.00	1.00	1.00	1.00	.999	1.00	.963	.991	.997	.995	.985	.971	.934	.778	.990	1.00	.977	1.00	.999	.996	.989	.984	.938	.993	.989
2.0	.50	.992	1.00	1.00	1.00	.999	.996	.968	1.00	.993	.992	.992	.988	.984	.970	.936	.796	.989	1.00	.993	.996	.995	.992	.980	.969	.878	.992	.997
2.0	.90	.998	.975	.969	.953	.885	.818	.570	.933	.995	.997	.981	.972	.936	.887	.807	.563	.914	.999	.996	.975	.965	.939	.891	.812	.572	.920	.999

C=6 N=12 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.286	.333	.254	.169	.085	.035	.004	.092	.242	.506	.390	.295	.199	.095	.047	.008	.353	.988	.365	.322	.259	.173	.081	.040	.008	.152	.696
0.5	.50	.313	.331	.251	.171	.087	.044	.012	.166	.696	.550	.415	.336	.231	.108	.058	.011	.402	.994	.438	.371	.285	.196	.099	.051	.008	.273	.928
0.5	.90	.511	.388	.301	.210	.118	.053	.016	.487	.987	.586	.401	.309	.220	.122	.057	.008	.465	.988	.564	.408	.297	.203	.089	.049	.009	.463	.973
2.0	.00	.982	1.00	1.00	1.00	1.00	1.00	.996	1.00	.962	.985	.983	.975	.956	.927	.879	.676	.974	1.00	.978	.997	.995	.994	.985	.968	.889	.992	.990
2.0	.50	.988	.999	.999	.998	.995	.989	.934	.998	.990	.981	.978	.969	.953	.910	.843	.643	.975	1.00	.987	.994	.992	.983	.969	.937	.800	.989	.998
2.0	.90	.993	.974	.962	.939	.878	.791	.559	.913	.999	.991	.965	.941	.919	.858	.762	.498	.899	.996	.995	.972	.958	.928	.861	.778	.506	.901	1.00

C=6 N=16 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.084	.393	.302	.206	.104	.062	.006	.111	.000	.042	.398	.296	.197	.100	.049	.012	.121	.015	.044	.396	.314	.213	.104	.057	.009	.124	.004
0.5	.50	.033	.410	.305	.212	.112	.060	.012	.206	.214	.022	.373	.292	.184	.097	.057	.015	.228	.284	.010	.395	.301	.185	.098	.036	.011	.224	.288
2.0	.00	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.977	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.996	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.992
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.999

C=6 N=16 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.180	.373	.284	.195	.112	.061	.014	.117	.011	.138	.403	.315	.220	.107	.056	.013	.190	.221	.182	.394	.308	.201	.107	.060	.016	.140	.066
0.5	.50	.168	.406	.315	.216	.104	.058	.017	.213	.292	.134	.370	.269	.198	.104	.058	.014	.299	.572	.143	.399	.297	.199	.103	.065	.013	.303	.522
0.5	.75	.086	.414	.302	.215	.118	.060	.020	.838	.946	.066	.385	.289	.194	.105	.053	.017	.815	.956	.063	.409	.315	.218	.094	.052	.016	.812	.942
2.0	.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.972	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.999	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.988
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.998	.999	1.00	1.00	1.00	1.00	1.00	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
2.0	.75	1.00	1.00	1.00	1.00	1.00	1.00	.996	1.00	1.00	1.00	1.00	1.00	1.00	.999	.999	.996	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.995	1.00	1.00

C=6 N=16 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.255	.377	.281	.195	.097	.048	.010	.105	.029	.308	.404	.302	.203	.097	.048	.009	.263	.666	.304	.393	.316	.209	.109	.054	.009	.155	.219
0.5	.50	.251	.359	.272	.187	.087	.039	.007	.190	.387	.293	.380	.292	.196	.101	.046	.017	.364	.839	.291	.395	.297	.207	.101	.056	.013	.316	.717
0.5	.85	.196	.392	.304	.214	.107	.061	.018	.861	.999	.200	.371	.276	.180	.085	.046	.009	.871	1.00	.225	.433	.330	.225	.129	.074	.015	.869	1.00
2.0	.00	.996	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.965	.998	1.00	1.00	1.00	1.00	.999	.994	1.00	.999	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.991
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	.998	1.00	.994	.999	1.00	1.00	1.00	.999	.996	.985	1.00	1.00	.998	1.00	1.00	1.00	.999	.999	.994	1.00	.998
2.0	.85	.999	1.00	.999	.999	.994	.986	.944	.999	1.00	.999	1.00	1.00	.998	.991	.985	.927	.997	1.00	1.00	.999	.998	.997	.992	.978	.923	.999	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=6 N=16 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.318	.369	.287	.198	.105	.048	.009	.112	.065	.434	.394	.304	.199	.100	.053	.009	.374	.896	.397	.381	.295	.201	.112	.071	.014	.175	.404
0.5	.50	.338	.356	.281	.196	.098	.052	.010	.209	.515	.434	.408	.308	.202	.093	.051	.011	.448	.954	.439	.381	.305	.214	.103	.053	.011	.328	.835
0.5	.85	.418	.407	.298	.205	.107	.052	.012	.772	1.00	.423	.393	.310	.214	.105	.052	.012	.748	1.00	.438	.418	.334	.236	.115	.054	.009	.762	1.00
2.0	.00	.999	1.00	1.00	1.00	1.00	1.00	.999	1.00	.964	.998	1.00	.998	.997	.996	.993	.967	1.00	1.00	.998	1.00	1.00	1.00	1.00	1.00	.998	1.00	.992
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.997	.999	.999	.998	.998	.995	.990	.955	1.00	1.00	.998	1.00	1.00	.999	.999	.998	.981	1.00	.999
2.0	.85	.998	.998	.996	.993	.985	.970	.895	.996	1.00	1.00	.997	.995	.991	.983	.957	.872	.995	1.00	.999	.999	.997	.991	.978	.958	.882	.997	1.00

C=6 N=16 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.347	.347	.287	.201	.112	.052	.007	.126	.102	.547	.405	.297	.207	.112	.056	.011	.417	.968	.437	.386	.306	.217	.111	.056	.015	.192	.536
0.5	.50	.392	.360	.286	.206	.099	.060	.011	.206	.569	.563	.394	.297	.218	.135	.071	.015	.458	.983	.491	.382	.287	.215	.101	.056	.017	.326	.901
0.5	.90	.563	.390	.275	.185	.105	.050	.006	.607	.991	.546	.403	.301	.213	.109	.055	.017	.615	.998	.539	.383	.296	.198	.108	.055	.007	.608	.994
2.0	.00	.993	1.00	1.00	1.00	1.00	1.00	.998	1.00	.962	.999	.999	.999	.996	.987	.974	.899	.998	.999	1.00	1.00	1.00	1.00	1.00	.999	.990	1.00	.995
2.0	.50	.999	1.00	1.00	1.00	.999	.997	.989	1.00	.996	.997	.997	.996	.994	.981	.967	.891	.998	1.00	.997	.999	.998	.998	.995	.989	.946	1.00	1.00
2.0	.90	.998	.989	.982	.977	.945	.911	.751	.956	.999	.999	.995	.990	.976	.945	.907	.726	.954	.998	.998	.986	.980	.969	.944	.912	.727	.958	1.00

C=6 N=16 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.386	.345	.267	.192	.108	.067	.010	.119	.152	.606	.386	.289	.194	.099	.060	.011	.402	.987	.496	.366	.285	.204	.095	.042	.008	.184	.620
0.5	.50	.404	.333	.247	.163	.091	.045	.007	.200	.595	.652	.435	.335	.230	.128	.068	.014	.481	.995	.547	.390	.303	.217	.103	.060	.007	.329	.926
0.5	.90	.642	.395	.308	.205	.102	.053	.015	.546	.994	.647	.407	.308	.208	.114	.056	.013	.538	.983	.670	.407	.302	.215	.114	.059	.012	.511	.981
2.0	.00	.993	1.00	1.00	1.00	1.00	1.00	.999	1.00	.958	.994	.995	.990	.979	.952	.929	.810	.992	1.00	.999	1.00	1.00	.999	.999	.996	.971	.999	.993
2.0	.50	1.00	1.00	1.00	1.00	1.00	.999	.990	1.00	1.00	.998	.990	.987	.978	.950	.923	.791	.989	1.00	.996	.999	.998	.998	.989	.974	.901	.997	.998
2.0	.90	.998	.986	.981	.960	.927	.872	.703	.945	1.00	.996	.982	.973	.962	.922	.860	.668	.947	.997	.999	.981	.967	.956	.913	.857	.655	.938	.999

C=9 N=4 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.006	.368	.275	.188	.107	.067	.029	.091	.468	.001	.384	.301	.187	.118	.072	.038	.115	.645	.003	.402	.292	.200	.102	.062	.028	.092	.603
0.5	.50	.003	.370	.279	.180	.103	.071	.040	.095	.610	.002	.385	.290	.213	.130	.084	.043	.125	.660	.001	.423	.336	.224	.130	.087	.045	.114	.710
2.0	.00	.864	1.00	1.00	1.00	1.00	1.00	.981	1.00	.972	.889	1.00	1.00	1.00	.998	.993	.905	.999	.981	.881	1.00	1.00	1.00	1.00	.996	.947	1.00	.984
2.0	.50	.903	.999	.998	.998	.996	.984	.910	.998	.985	.905	1.00	.999	.999	.995	.980	.869	.997	.980	.886	1.00	.998	.997	.985	.963	.836	.994	.987

C=9 N=4 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.025	.355	.267	.195	.102	.064	.028	.102	.619	.014	.382	.286	.197	.120	.069	.031	.118	.795	.018	.368	.283	.204	.117	.070	.026	.112	.716
0.5	.50	.014	.377	.295	.206	.114	.067	.029	.109	.724	.019	.398	.308	.213	.120	.081	.041	.132	.809	.008	.380	.287	.211	.117	.066	.034	.119	.803
0.5	.75	.011	.405	.297	.211	.129	.082	.045	.199	.825	.005	.395	.297	.213	.123	.075	.045	.198	.856	.006	.397	.306	.199	.126	.090	.042	.176	.834
2.0	.00	.845	1.00	1.00	1.00	1.00	1.00	.946	1.00	.968	.856	.999	.998	.997	.985	.954	.777	.994	.986	.852	.999	.999	.998	.998	.980	.858	.997	.982
2.0	.50	.866	1.00	.999	.999	.990	.967	.828	.995	.987	.869	.997	.995	.993	.982	.934	.723	.990	.984	.879	.998	.995	.989	.969	.930	.722	.981	.981
2.0	.75	.906	.993	.983	.975	.932	.856	.662	.994	.991	.903	.993	.989	.974	.924	.828	.644	.989	.993	.885	.991	.985	.974	.915	.814	.598	.988	.994

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=9 N=4 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.053	.344	.265	.188	.107	.060	.022	.109	.683	.028	.379	.279	.184	.082	.051	.023	.111	.877	.061	.384	.303	.212	.107	.065	.029	.118	.802
0.5	.50	.037	.359	.286	.198	.103	.056	.022	.102	.806	.039	.374	.284	.199	.101	.051	.019	.144	.902	.056	.390	.312	.202	.095	.054	.024	.130	.872
0.5	.85	.018	.366	.280	.201	.101	.060	.030	.344	.910	.014	.367	.276	.187	.107	.071	.045	.344	.897	.021	.411	.313	.230	.135	.088	.043	.390	.925
2.0	.00	.824	.999	.999	.999	.999	.994	.910	.999	.970	.857	.994	.990	.984	.956	.871	.604	.968	.994	.811	.999	.998	.992	.976	.928	.720	.980	.978
2.0	.50	.820	.998	.995	.990	.975	.914	.717	.984	.983	.873	.992	.986	.978	.930	.843	.583	.967	.992	.844	.992	.985	.977	.941	.863	.618	.966	.988
2.0	.85	.895	.976	.967	.924	.824	.620	.359	.973	.992	.881	.975	.956	.908	.807	.642	.402	.968	.997	.908	.976	.951	.922	.812	.651	.373	.968	.998

C=9 N=4 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.065	.333	.259	.190	.111	.066	.025	.116	.728	.084	.380	.301	.200	.095	.042	.015	.153	.917	.074	.354	.280	.184	.091	.045	.015	.106	.843
0.5	.50	.065	.342	.270	.186	.095	.054	.020	.115	.840	.077	.376	.291	.195	.095	.046	.013	.166	.936	.084	.373	.284	.202	.112	.059	.022	.155	.905
0.5	.85	.074	.409	.297	.194	.101	.063	.029	.336	.945	.080	.406	.309	.194	.106	.064	.031	.336	.958	.064	.361	.269	.180	.103	.069	.040	.333	.955
2.0	.00	.810	1.00	1.00	.998	.998	.991	.844	.997	.967	.830	.972	.959	.934	.863	.758	.465	.917	.992	.830	.987	.982	.975	.949	.886	.633	.954	.983
2.0	.50	.817	.992	.991	.986	.956	.886	.648	.967	.980	.836	.966	.953	.925	.856	.727	.428	.926	.990	.846	.984	.980	.963	.915	.825	.530	.946	.991
2.0	.85	.846	.956	.918	.879	.761	.598	.362	.954	.991	.867	.953	.931	.885	.757	.596	.300	.949	.996	.875	.955	.930	.872	.759	.587	.318	.940	.995

C=9 N=4 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.075	.332	.265	.181	.111	.063	.021	.118	.748	.126	.363	.281	.187	.100	.049	.019	.177	.950	.115	.346	.270	.181	.097	.049	.018	.124	.861
0.5	.50	.094	.343	.260	.190	.105	.055	.019	.124	.859	.117	.380	.283	.193	.103	.054	.023	.199	.953	.110	.356	.275	.188	.086	.046	.021	.143	.903
0.5	.90	.114	.385	.296	.197	.105	.060	.033	.406	.963	.106	.388	.287	.184	.085	.049	.026	.417	.967	.112	.381	.275	.192	.083	.046	.024	.415	.965
2.0	.00	.760	1.00	1.00	.999	.996	.974	.809	.997	.959	.818	.944	.926	.893	.816	.685	.331	.880	.991	.784	.983	.979	.967	.912	.839	.530	.930	.967
2.0	.50	.800	.995	.993	.977	.937	.858	.575	.955	.988	.819	.941	.916	.879	.787	.627	.327	.892	.997	.802	.968	.953	.928	.862	.728	.436	.923	.992
2.0	.90	.882	.922	.891	.826	.681	.500	.199	.874	.976	.869	.910	.879	.820	.657	.460	.186	.852	.970	.865	.901	.873	.814	.652	.459	.175	.855	.968

C=9 N=4 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.098	.327	.246	.166	.088	.041	.006	.101	.783	.149	.352	.262	.174	.086	.042	.010	.186	.962	.131	.326	.260	.172	.077	.035	.006	.108	.905
0.5	.50	.102	.343	.259	.174	.097	.053	.017	.114	.872	.152	.368	.281	.184	.092	.043	.019	.207	.971	.125	.350	.267	.187	.088	.042	.010	.155	.943
0.5	.90	.151	.375	.282	.192	.091	.060	.027	.366	.963	.159	.394	.307	.194	.102	.058	.026	.383	.963	.149	.365	.278	.179	.082	.043	.024	.379	.969
2.0	.00	.754	1.00	.999	.994	.985	.959	.738	.990	.958	.798	.913	.882	.848	.741	.592	.258	.842	.995	.764	.973	.960	.931	.862	.774	.443	.889	.982
2.0	.50	.780	.982	.976	.951	.904	.826	.530	.934	.981	.773	.898	.862	.816	.702	.554	.247	.830	.994	.776	.938	.909	.880	.797	.657	.323	.845	.987
2.0	.90	.797	.872	.835	.765	.620	.430	.164	.831	.978	.832	.872	.835	.779	.632	.434	.172	.822	.971	.841	.890	.847	.794	.618	.420	.165	.838	.983

C=9 N=6 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.013	.366	.275	.180	.093	.045	.018	.088	.112	.003	.412	.303	.207	.114	.071	.024	.113	.240	.006	.380	.295	.199	.099	.062	.025	.097	.185
0.5	.50	.007	.403	.302	.204	.107	.059	.017	.117	.293	.001	.404	.324	.220	.120	.072	.025	.120	.302	.001	.390	.292	.200	.103	.062	.024	.104	.333
2.0	.00	.944	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.964	.964	1.00	1.00	1.00	1.00	.999	.994	1.00	.988	.969	1.00	1.00	1.00	1.00	1.00	.997	1.00	.985
2.0	.50	.963	1.00	1.00	1.00	1.00	1.00	.991	1.00	.990	.976	1.00	1.00	1.00	1.00	.997	.974	1.00	.995	.973	1.00	1.00	1.00	1.00	.998	.969	1.00	.997

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=9 N=6 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.044	.369	.279	.197	.115	.061	.015	.112	.253	.023	.378	.284	.190	.108	.061	.029	.118	.511	.027	.372	.285	.191	.096	.053	.018	.105	.428
0.5	.50	.032	.376	.278	.191	.100	.060	.024	.115	.464	.014	.401	.302	.194	.085	.052	.022	.120	.601	.014	.371	.286	.200	.109	.065	.026	.130	.559
0.5	.75	.006	.399	.307	.207	.110	.069	.027	.253	.656	.012	.388	.296	.210	.111	.068	.025	.247	.651	.009	.391	.300	.191	.111	.070	.028	.245	.689
2.0	.00	.945	1.00	1.00	1.00	1.00	1.00	.998	1.00	.967	.950	1.00	1.00	1.00	.999	.999	.960	.999	.989	.953	1.00	1.00	1.00	1.00	1.00	.989	1.00	.984
2.0	.50	.963	1.00	1.00	1.00	1.00	.997	.969	1.00	.991	.964	1.00	.999	.999	.995	.990	.923	.999	.994	.957	1.00	1.00	1.00	.997	.987	.910	1.00	.990
2.0	.75	.979	1.00	1.00	.996	.986	.968	.837	1.00	.998	.964	.999	.997	.992	.980	.953	.819	.999	.993	.972	.999	.997	.996	.985	.965	.812	.999	.996

C=9 N=6 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.062	.327	.236	.164	.082	.038	.009	.086	.356	.051	.363	.291	.179	.099	.049	.010	.141	.740	.070	.401	.316	.212	.110	.059	.016	.119	.577
0.5	.50	.069	.371	.286	.191	.108	.052	.019	.121	.570	.059	.403	.294	.200	.101	.056	.016	.172	.790	.066	.385	.298	.205	.096	.053	.017	.138	.715
0.5	.85	.041	.420	.325	.207	.111	.063	.028	.528	.873	.026	.419	.331	.224	.118	.075	.033	.543	.856	.034	.401	.306	.211	.122	.070	.030	.520	.871
2.0	.00	.918	1.00	1.00	1.00	1.00	1.00	.995	1.00	.959	.949	.999	.999	.995	.988	.966	.851	.993	.988	.936	1.00	1.00	.999	.998	.998	.950	.998	.982
2.0	.50	.929	1.00	1.00	1.00	.998	.990	.928	.999	.980	.949	.996	.994	.991	.979	.948	.781	.988	.993	.948	.999	.999	.997	.987	.961	.823	.992	.991
2.0	.85	.964	.990	.983	.971	.918	.841	.581	.986	.999	.975	.992	.986	.979	.938	.862	.595	.987	.999	.957	.989	.981	.971	.920	.851	.588	.983	1.00

C=9 N=6 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.084	.330	.254	.186	.099	.042	.005	.106	.409	.131	.390	.305	.189	.101	.048	.017	.171	.856	.128	.367	.290	.189	.097	.050	.011	.125	.699
0.5	.50	.101	.353	.271	.192	.106	.050	.014	.128	.622	.098	.363	.283	.188	.088	.043	.017	.197	.889	.122	.403	.301	.196	.113	.057	.013	.156	.812
0.5	.85	.105	.406	.305	.194	.096	.052	.018	.458	.930	.102	.415	.331	.208	.106	.053	.019	.448	.953	.103	.393	.289	.198	.091	.044	.013	.424	.956
2.0	.00	.907	1.00	1.00	1.00	1.00	.999	.982	1.00	.955	.939	.990	.983	.978	.953	.913	.695	.967	.993	.919	.998	.997	.996	.990	.978	.879	.991	.983
2.0	.50	.932	1.00	.999	.999	.993	.978	.873	.998	.986	.941	.994	.990	.985	.955	.900	.669	.985	.996	.927	.996	.993	.989	.964	.931	.753	.981	.993
2.0	.85	.950	.984	.971	.953	.890	.792	.521	.978	.998	.952	.983	.969	.945	.892	.802	.502	.976	1.00	.956	.979	.969	.946	.892	.795	.518	.974	1.00

C=9 N=6 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.122	.343	.278	.185	.096	.043	.005	.106	.482	.165	.364	.278	.176	.078	.037	.002	.197	.934	.137	.325	.255	.185	.085	.040	.011	.116	.730
0.5	.50	.118	.353	.271	.177	.086	.038	.010	.121	.691	.171	.362	.294	.197	.104	.053	.013	.237	.929	.152	.351	.274	.176	.097	.054	.012	.167	.864
0.5	.90	.165	.395	.307	.208	.103	.063	.020	.527	.974	.156	.392	.299	.212	.113	.059	.021	.510	.979	.159	.386	.285	.193	.088	.055	.019	.512	.982
2.0	.00	.888	1.00	1.00	1.00	.998	.994	.963	.998	.959	.935	.985	.976	.961	.916	.845	.561	.950	.997	.910	.995	.994	.989	.979	.959	.785	.984	.980
2.0	.50	.919	.998	.998	.997	.985	.971	.867	.990	.973	.925	.978	.965	.945	.894	.815	.511	.944	.996	.910	.980	.977	.965	.933	.890	.655	.957	.982
2.0	.90	.961	.965	.944	.906	.819	.710	.370	.931	.998	.950	.956	.929	.881	.799	.665	.353	.917	.994	.971	.959	.930	.896	.807	.670	.314	.920	.997

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=9 N=6 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.134	.323	.261	.182	.103	.059	.010	.112	.535	.221	.358	.275	.191	.086	.025	.007	.232	.955	.200	.371	.289	.194	.088	.047	.008	.129	.777
0.5	.50	.148	.321	.260	.193	.116	.058	.012	.151	.756	.250	.390	.321	.218	.105	.048	.007	.277	.968	.176	.349	.271	.176	.083	.031	.004	.166	.889
0.5	.90	.229	.372	.286	.202	.088	.041	.011	.454	.986	.266	.404	.294	.192	.104	.039	.011	.452	.989	.232	.372	.270	.190	.088	.050	.010	.419	.986
2.0	.00	.889	1.00	1.00	1.00	1.00	.998	.947	1.00	.956	.882	.950	.929	.901	.825	.723	.381	.906	.993	.887	.991	.988	.978	.952	.916	.687	.960	.975
2.0	.50	.891	.998	.997	.994	.969	.944	.764	.983	.981	.911	.959	.945	.915	.856	.759	.447	.936	.997	.909	.980	.971	.957	.913	.854	.591	.948	.992
2.0	.90	.931	.941	.912	.872	.791	.672	.331	.914	.996	.932	.933	.914	.872	.762	.630	.285	.905	.997	.937	.941	.919	.879	.787	.639	.278	.910	.998

C=9 N=9 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.028	.411	.305	.201	.110	.060	.017	.107	.012	.006	.412	.315	.205	.113	.066	.018	.121	.046	.004	.372	.278	.184	.094	.047	.024	.091	.026
0.5	.50	.003	.382	.281	.201	.097	.057	.017	.107	.084	.000	.406	.295	.200	.120	.068	.021	.138	.118	.002	.388	.287	.190	.102	.053	.012	.116	.136
2.0	.00	.991	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.974	.993	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.989	.986	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.982
2.0	.50	.993	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.992	.993	1.00	1.00	1.00	1.00	1.00	.999	1.00	.992	.996	1.00	1.00	1.00	1.00	1.00	.999	1.00	.998

C=9 N=9 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.064	.379	.283	.196	.112	.056	.019	.119	.065	.025	.388	.283	.187	.089	.043	.012	.114	.273	.047	.380	.284	.191	.094	.053	.009	.101	.164
0.5	.50	.052	.380	.294	.204	.105	.059	.014	.130	.242	.029	.397	.284	.195	.103	.061	.019	.162	.397	.023	.395	.301	.206	.111	.060	.021	.153	.328
0.5	.75	.016	.404	.293	.199	.109	.064	.017	.395	.598	.016	.397	.307	.210	.117	.068	.014	.384	.629	.011	.397	.302	.202	.103	.056	.024	.367	.619
2.0	.00	.977	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.959	.992	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.993	.977	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.978
2.0	.50	.992	1.00	1.00	1.00	1.00	.999	.997	1.00	.992	.994	1.00	1.00	1.00	.998	.998	.994	.999	.995	.990	1.00	1.00	1.00	1.00	1.00	.992	1.00	.992
2.0	.75	.994	1.00	1.00	1.00	1.00	.998	.966	1.00	.998	.991	.999	.999	.999	.998	.994	.966	1.00	.996	.995	1.00	1.00	1.00	.999	.994	.970	1.00	.999

C=9 N=9 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.089	.361	.286	.191	.097	.052	.008	.103	.127	.076	.368	.270	.181	.095	.051	.012	.159	.566	.118	.381	.303	.194	.111	.057	.014	.128	.349
0.5	.50	.081	.361	.280	.175	.091	.049	.012	.127	.348	.080	.384	.282	.184	.104	.050	.024	.182	.654	.090	.401	.304	.212	.112	.062	.018	.185	.586
0.5	.85	.040	.432	.330	.211	.096	.056	.016	.727	.912	.047	.388	.284	.189	.100	.062	.023	.702	.903	.046	.400	.311	.207	.119	.055	.019	.728	.914
2.0	.00	.979	1.00	1.00	1.00	1.00	1.00	.999	1.00	.968	.986	1.00	1.00	1.00	.999	.997	.977	1.00	.992	.987	1.00	1.00	1.00	1.00	1.00	.999	1.00	.987
2.0	.50	.978	1.00	1.00	1.00	1.00	1.00	.991	1.00	.984	.988	1.00	1.00	.999	.998	.994	.955	.998	.993	.985	1.00	1.00	1.00	1.00	.998	.973	1.00	.993
2.0	.85	.994	.998	.996	.992	.981	.960	.842	1.00	.999	.994	.999	.998	.997	.982	.959	.832	.999	1.00	.996	.998	.996	.994	.982	.962	.839	.998	.999

C=9 N=9 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.144	.336	.255	.177	.089	.057	.015	.093	.191	.171	.359	.271	.196	.098	.057	.014	.214	.788	.167	.367	.282	.190	.082	.036	.008	.116	.457
0.5	.50	.140	.377	.284	.186	.095	.043	.013	.139	.484	.164	.388	.291	.194	.091	.041	.005	.228	.847	.176	.384	.278	.189	.097	.046	.011	.186	.727
0.5	.85	.152	.413	.324	.225	.114	.065	.016	.596	.933	.151	.404	.304	.201	.106	.059	.021	.609	.959	.141	.404	.306	.202	.106	.049	.017	.604	.967
2.0	.00	.979	1.00	1.00	1.00	1.00	1.00	.998	1.00	.969	.981	.998	.997	.993	.984	.972	.909	.991	.997	.977	1.00	1.00	.999	.997	.995	.980	.997	.989
2.0	.50	.986	1.00	1.00	1.00	.999	.998	.988	.999	.986	.988	.999	.998	.997	.992	.979	.890	.998	.999	.976	1.00	.999	.998	.993	.989	.943	.997	.993
2.0	.85	.993	.999	.995	.983	.968	.927	.781	.999	1.00	.990	.997	.991	.982	.963	.931	.757	.997	1.00	.989	.993	.992	.979	.959	.925	.751	.994	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=9 N=9 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.156	.358	.271	.179	.088	.046	.006	.096	.250	.221	.372	.287	.201	.111	.048	.015	.254	.887	.192	.357	.276	.197	.092	.043	.010	.132	.594
0.5	.50	.169	.369	.270	.179	.095	.055	.007	.135	.525	.241	.387	.291	.183	.102	.051	.007	.288	.921	.228	.357	.282	.201	.097	.043	.004	.196	.796
0.5	.90	.232	.378	.297	.199	.096	.046	.010	.656	.994	.241	.420	.313	.191	.099	.047	.010	.667	.995	.246	.398	.311	.220	.106	.055	.014	.652	.990
2.0	.00	.964	1.00	1.00	1.00	1.00	1.00	.996	1.00	.954	.971	.996	.995	.985	.966	.932	.802	.989	.994	.968	1.00	1.00	.999	.994	.991	.956	.995	.976
2.0	.50	.968	1.00	1.00	.999	.998	.992	.967	.998	.991	.983	.994	.992	.985	.963	.937	.787	.990	1.00	.968	.999	.996	.995	.983	.972	.898	.995	.993
2.0	.90	.993	.988	.976	.963	.926	.849	.621	.974	1.00	.987	.981	.971	.959	.921	.847	.605	.966	.999	.990	.984	.975	.948	.909	.834	.591	.966	1.00

C=9 N=9 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.177	.354	.269	.190	.102	.058	.015	.113	.295	.320	.404	.310	.222	.121	.054	.013	.337	.970	.268	.368	.291	.204	.113	.049	.011	.160	.689
0.5	.50	.186	.321	.240	.173	.085	.040	.006	.127	.558	.321	.385	.301	.211	.105	.055	.009	.354	.962	.319	.393	.311	.221	.118	.053	.012	.232	.839
0.5	.90	.294	.375	.293	.202	.096	.046	.009	.592	.996	.308	.385	.286	.201	.109	.062	.015	.559	.996	.308	.373	.276	.179	.074	.037	.010	.543	.993
2.0	.00	.956	1.00	1.00	1.00	1.00	1.00	.995	1.00	.959	.965	.988	.976	.963	.938	.893	.699	.977	1.00	.957	1.00	.999	.993	.990	.980	.905	.991	.989
2.0	.50	.959	1.00	1.00	.998	.991	.986	.941	.997	.979	.971	.989	.980	.966	.951	.891	.693	.977	.999	.968	.998	.996	.988	.978	.955	.835	.988	.992
2.0	.90	.984	.983	.969	.949	.890	.809	.520	.968	1.00	.980	.966	.957	.936	.879	.796	.538	.949	.999	.983	.976	.966	.938	.871	.779	.492	.960	.999

C=9 N=12 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.025	.397	.293	.196	.100	.053	.013	.104	.000	.005	.375	.280	.181	.102	.059	.018	.111	.006	.010	.388	.290	.209	.096	.053	.010	.103	.002
0.5	.50	.004	.380	.291	.197	.117	.063	.009	.136	.041	.001	.366	.262	.170	.083	.049	.017	.102	.071	.003	.422	.321	.200	.108	.056	.022	.136	.075
2.0	.00	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.974	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.989	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.985
2.0	.50	.996	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.987	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.994	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.994

C=9 N=12 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.091	.391	.293	.207	.113	.060	.019	.120	.015	.049	.412	.324	.225	.115	.061	.016	.147	.117	.057	.384	.284	.194	.107	.060	.019	.126	.041
0.5	.50	.067	.407	.308	.216	.107	.056	.017	.140	.113	.036	.426	.321	.214	.107	.065	.016	.170	.262	.042	.396	.311	.218	.108	.064	.013	.168	.219
0.5	.75	.018	.394	.293	.197	.107	.049	.012	.459	.625	.022	.371	.282	.176	.095	.058	.014	.442	.624	.013	.412	.310	.208	.107	.054	.016	.509	.650
2.0	.00	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.976	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.994	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.986
2.0	.50	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.991	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.996	.996	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.997
2.0	.75	.998	1.00	1.00	1.00	1.00	1.00	.992	1.00	1.00	.998	1.00	1.00	1.00	1.00	.999	.992	1.00	1.00	.999	1.00	1.00	1.00	.999	.999	.994	1.00	.999

C=9 N=12 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.144	.391	.306	.202	.113	.056	.013	.120	.045	.119	.406	.317	.219	.103	.051	.009	.179	.457	.149	.396	.287	.201	.118	.059	.015	.137	.154
0.5	.50	.134	.388	.290	.198	.112	.058	.009	.151	.226	.097	.381	.273	.183	.089	.045	.009	.214	.584	.131	.384	.297	.183	.093	.049	.010	.194	.440
0.5	.85	.077	.423	.330	.227	.102	.054	.009	.870	.959	.054	.392	.307	.184	.099	.051	.010	.858	.968	.069	.404	.306	.209	.108	.065	.014	.837	.955
2.0	.00	.992	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.971	.998	1.00	1.00	1.00	1.00	1.00	.999	1.00	.996	.994	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.984
2.0	.50	.991	1.00	1.00	1.00	1.00	1.00	.998	1.00	.984	.996	1.00	1.00	1.00	.999	.999	.996	1.00	.999	.997	1.00	1.00	1.00	1.00	1.00	.996	1.00	.996
2.0	.85	1.00	1.00	1.00	1.00	1.00	.992	.953	1.00	1.00	.998	.999	.999	.997	.995	.991	.954	1.00	1.00	.999	.998	.998	.997	.995	.987	.932	.998	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=9 N=12 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.150	.356	.260	.184	.089	.038	.007	.101	.073	.234	.406	.318	.211	.117	.055	.015	.268	.745	.222	.385	.302	.205	.107	.048	.012	.145	.349
0.5	.50	.176	.350	.264	.160	.087	.050	.009	.127	.297	.233	.405	.309	.223	.123	.057	.012	.309	.822	.237	.382	.305	.208	.098	.053	.014	.209	.624
0.5	.85	.174	.413	.317	.220	.123	.068	.012	.752	.977	.188	.400	.299	.206	.111	.056	.010	.728	.974	.180	.406	.296	.192	.094	.051	.010	.730	.980
2.0	.00	.996	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.968	.995	1.00	1.00	1.00	1.00	.998	.971	1.00	.997	.992	1.00	1.00	1.00	1.00	1.00	.998	1.00	.989
2.0	.50	.992	1.00	1.00	1.00	1.00	1.00	.999	1.00	.989	.998	.999	.999	.999	.997	.993	.967	.999	.999	.996	1.00	1.00	.999	.998	.995	.981	1.00	.998
2.0	.85	.999	1.00	.998	.995	.983	.976	.908	.999	1.00	.995	.995	.995	.995	.989	.980	.905	.996	1.00	.998	1.00	.999	.996	.991	.976	.898	1.00	1.00

C=9 N=12 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.215	.378	.308	.208	.105	.047	.010	.122	.152	.338	.384	.308	.207	.102	.054	.008	.342	.892	.288	.383	.284	.197	.089	.043	.009	.144	.449
0.5	.50	.237	.372	.288	.201	.097	.048	.011	.160	.400	.303	.378	.293	.175	.090	.047	.006	.359	.921	.305	.388	.310	.224	.106	.057	.012	.242	.738
0.5	.90	.293	.392	.303	.202	.109	.058	.010	.772	.997	.289	.397	.309	.203	.094	.034	.009	.753	.998	.317	.409	.300	.207	.113	.066	.015	.744	1.00
2.0	.00	.988	1.00	1.00	1.00	1.00	1.00	.998	1.00	.953	.990	1.00	.999	.993	.986	.980	.917	.996	.999	.994	1.00	1.00	1.00	.999	.998	.993	1.00	.988
2.0	.50	.990	1.00	1.00	1.00	1.00	.999	.991	1.00	.990	.995	.999	.999	.996	.987	.976	.895	.995	.998	.989	1.00	.999	.999	.998	.995	.962	.998	.994
2.0	.90	.998	.989	.986	.979	.962	.933	.787	.984	1.00	.998	.994	.989	.983	.958	.921	.766	.988	1.00	.999	.997	.993	.987	.960	.931	.772	.994	1.00

C=9 N=12 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.225	.334	.261	.180	.087	.036	.004	.097	.149	.410	.397	.323	.219	.112	.059	.012	.374	.949	.309	.359	.262	.171	.084	.043	.005	.139	.555
0.5	.50	.279	.368	.286	.208	.107	.050	.006	.153	.476	.372	.371	.273	.195	.092	.041	.013	.379	.967	.360	.383	.288	.192	.103	.045	.007	.255	.821
0.5	.90	.389	.401	.294	.214	.111	.063	.017	.687	.997	.428	.412	.323	.212	.101	.058	.011	.664	.999	.429	.415	.312	.217	.116	.057	.012	.678	.998
2.0	.00	.987	1.00	1.00	1.00	1.00	1.00	.999	1.00	.961	.992	.997	.992	.990	.970	.944	.841	.994	1.00	.990	1.00	.999	.999	.999	.998	.972	.999	.994
2.0	.50	.992	1.00	1.00	1.00	1.00	.999	.994	1.00	.986	.990	.991	.990	.988	.972	.948	.832	.992	1.00	.992	.999	.998	.996	.995	.988	.920	.997	.996
2.0	.90	.997	.993	.986	.977	.953	.903	.746	.987	1.00	1.00	.996	.990	.980	.955	.907	.712	.991	1.00	.994	.989	.981	.971	.940	.892	.720	.986	1.00

C=9 N=16 CV=1.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.052	.412	.318	.213	.100	.052	.010	.110	.000	.004	.390	.313	.205	.099	.053	.008	.117	.000	.020	.415	.306	.212	.110	.050	.009	.131	.000
0.5	.50	.010	.388	.286	.181	.102	.058	.014	.139	.038	.005	.378	.288	.193	.091	.042	.011	.146	.051	.009	.397	.304	.200	.108	.055	.015	.148	.040
2.0	.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.978	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.990	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.986
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.991	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.988	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.997

C=9 N=16 CV=2.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.091	.372	.283	.198	.103	.058	.014	.110	.002	.070	.393	.306	.191	.096	.043	.012	.137	.050	.064	.363	.263	.186	.091	.046	.008	.121	.005
0.5	.50	.077	.372	.287	.197	.111	.062	.019	.145	.059	.048	.374	.286	.187	.104	.065	.016	.204	.191	.058	.396	.311	.216	.103	.056	.015	.200	.156
0.5	.75	.020	.373	.295	.197	.105	.058	.014	.566	.701	.023	.394	.300	.208	.096	.047	.010	.567	.702	.023	.398	.311	.213	.114	.066	.020	.614	.735
2.0	.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.976	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.985
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.989	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.999
2.0	.75	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.998	1.00	1.00

Appendix I. SSL Simulation Results: Estimated Probabilities of Investigating Further

C=9 N=16 CV=2.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.163	.379	.281	.198	.113	.052	.008	.124	.012	.170	.397	.297	.199	.098	.054	.009	.216	.331	.170	.380	.279	.186	.103	.053	.013	.140	.066
0.5	.50	.187	.396	.306	.209	.113	.056	.019	.158	.121	.145	.388	.282	.190	.090	.048	.013	.269	.467	.161	.404	.301	.208	.105	.051	.008	.226	.330
0.5	.85	.071	.420	.322	.207	.098	.053	.014	.952	.984	.065	.438	.331	.232	.107	.062	.015	.963	.986	.085	.406	.304	.201	.106	.058	.018	.942	.988
2.0	.00	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.966	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.996	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.986
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.995	1.00	1.00	1.00	1.00	1.00	1.00	.999	1.00	1.00	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.996
2.0	.85	1.00	1.00	1.00	1.00	.998	.997	.982	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.998	.989	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.997	.983	1.00	1.00

C=9 N=16 CV=3.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.227	.400	.315	.210	.105	.053	.005	.125	.026	.279	.366	.269	.192	.099	.047	.007	.287	.655	.278	.383	.292	.205	.106	.057	.013	.170	.174
0.5	.50	.256	.390	.302	.224	.124	.049	.011	.184	.207	.297	.376	.291	.204	.104	.047	.007	.361	.766	.286	.399	.299	.192	.097	.060	.017	.271	.548
0.5	.85	.252	.387	.277	.186	.093	.050	.011	.860	.982	.225	.368	.282	.186	.093	.045	.011	.829	.991	.247	.430	.336	.229	.135	.074	.015	.851	.987
2.0	.00	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.961	.999	1.00	1.00	1.00	.999	.998	.997	.999	.997	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.989
2.0	.50	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.993	.999	1.00	1.00	1.00	1.00	1.00	.991	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
2.0	.85	1.00	1.00	1.00	.999	.997	.991	.971	1.00	1.00	1.00	1.00	1.00	1.00	.998	.993	.964	1.00	1.00	1.00	1.00	1.00	1.00	.996	.995	.968	1.00	1.00

C=9 N=16 CV=3.5

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.271	.365	.283	.202	.114	.071	.009	.130	.070	.392	.368	.276	.180	.085	.041	.010	.387	.867	.348	.374	.294	.201	.103	.056	.014	.166	.291
0.5	.50	.319	.353	.278	.190	.098	.058	.009	.162	.271	.382	.366	.282	.199	.097	.050	.013	.441	.918	.397	.419	.319	.220	.113	.052	.011	.295	.678
0.5	.90	.396	.432	.338	.224	.118	.058	.015	.846	1.00	.351	.387	.289	.198	.106	.044	.010	.822	1.00	.351	.411	.325	.223	.113	.061	.006	.843	1.00
2.0	.00	.995	1.00	1.00	1.00	1.00	1.00	1.00	1.00	.961	.999	1.00	1.00	1.00	1.00	.998	.976	1.00	1.00	.999	1.00	1.00	1.00	1.00	1.00	.999	1.00	.991
2.0	.50	.999	1.00	1.00	1.00	1.00	1.00	.999	1.00	.991	.998	1.00	1.00	1.00	.999	.993	.968	1.00	1.00	1.00	1.00	1.00	1.00	.999	.999	.994	.999	1.00
2.0	.90	1.00	.997	.996	.993	.985	.970	.902	.995	1.00	1.00	.999	.997	.997	.991	.975	.887	.999	1.00	1.00	.998	.996	.993	.980	.970	.881	.996	1.00

C=9 N=16 CV=4.0

MU	MIX	MxL	C40L	C30L	C20L	C10L	C05L	C01L	LfL	LoL	MxG	C40G	C30G	C20G	C10G	C05G	C01G	LfG	LoG	MxW	C40W	C30W	C20W	C10W	C05W	C01W	LfW	LoW
0.5	.00	.297	.353	.276	.202	.111	.052	.014	.125	.072	.502	.379	.282	.176	.088	.049	.010	.438	.949	.414	.358	.280	.183	.090	.039	.005	.165	.394
0.5	.50	.379	.393	.305	.209	.102	.053	.004	.181	.337	.513	.413	.325	.215	.116	.066	.015	.513	.967	.441	.377	.288	.207	.095	.046	.010	.293	.779
0.5	.90	.481	.402	.294	.198	.100	.049	.011	.793	1.00	.493	.387	.298	.201	.091	.047	.011	.738	.999	.493	.389	.315	.196	.102	.053	.010	.773	1.00
2.0	.00	.998	1.00	1.00	1.00	1.00	1.00	.999	1.00	.950	.996	.998	.998	.995	.991	.981	.932	.997	1.00	.998	1.00	1.00	1.00	1.00	1.00	.996	1.00	.994
2.0	.50	.997	1.00	1.00	1.00	1.00	1.00	.998	1.00	.990	.999	.998	.998	.995	.991	.982	.923	1.00	1.00	.997	1.00	1.00	1.00	.999	.997	.979	1.00	.999
2.0	.90	1.00	1.00	.997	.991	.979	.952	.872	.998	1.00	.999	.998	.995	.992	.970	.934	.817	.994	1.00	1.00	.998	.995	.986	.973	.939	.820	.994	1.00

APPENDIX J

Piazza Road Simulation Results

APPENDIX J

Piazza Road Simulation Results

Section 4.3.6 contains background information on the Piazza Road site and its seven exposure areas (EAs), as well as a complete description of the simulation setup and parameters. The following notation is used in the tables of this appendix.

EA = exposure area number (from 1 to 7)

MEAN = the true mean for the EA (an average of 96 measurements)

CV = the true value of the coefficient of variation for the EA

DES = indicator of whether compositing within strata (DES = W) or compositing across strata (DES = X) was used

C = the number of specimens per composite

N = the number of composite samples chemically analyzed.

The remaining four variables give the estimated error rates at 0.5 SSL and 2 SSL for the Max test (labelled as MAX 0.5SSL and MAX 2.0SSL) and the Chen test at the nominal .10 level (labelled as CHEN 0.5SSL and CHEN 2.0SSL).

Appendix J. Estimated decision error rates for Chen test at the 0.1 level, and Max test, for compositing within sector (DES=W) or across sector (DES=X), based on simulations from Piazza Road Data.

EA = EA # (1 to 7). MEAN and CV denote EA true mean and CV.
M = # of samples per composite. N = # of composite samples.

------------------------- EA=1 MEAN=2.1 CV=1.0 -------------------------

DES	M	N	MAX 0.5SSL	MAX 2.0SSL	CHEN 0.5SSL	CHEN 2.0SSL
W	4	4	.01	.03	.02	.00
X	4	4	.00	.12	.12	.00
W	4	6	.01	.01	.04	.00
X	4	6	.00	.04	.11	.00
W	4	8	.02	.00	.01	.00
X	4	8	.00	.01	.15	.00
W	6	4	.00	.01	.01	.00
X	6	4	.00	.11	.13	.00
W	6	6	.00	.01	.04	.00
X	6	6	.00	.04	.12	.00
W	6	8	.01	.00	.01	.00
X	6	8	.00	.01	.12	.00
W	8	4	.00	.02	.00	.00
X	8	4	.00	.09	.12	.00
W	8	6	.00	.01	.02	.00
X	8	6	.00	.04	.13	.00
W	8	8	.00	.00	.01	.00
X	8	8	.00	.02	.10	.00

------------------------- EA=2 MEAN=2.4 CV=1.6 -------------------------

DES	M	N	MAX 0.5SSL	MAX 2.0SSL	CHEN 0.5SSL	CHEN 2.0SSL
W	4	4	.07	.13	.08	.05
X	4	4	.04	.13	.11	.05
W	4	6	.09	.04	.05	.02
X	4	6	.05	.05	.11	.01
W	4	8	.11	.02	.05	.00
X	4	8	.07	.01	.11	.00
W	6	4	.04	.13	.09	.02
X	6	4	.01	.14	.09	.02
W	6	6	.05	.03	.04	.00
X	6	6	.01	.04	.09	.00
W	6	8	.06	.01	.04	.00
X	6	8	.01	.01	.13	.00
W	8	4	.03	.08	.09	.00
X	8	4	.00	.12	.10	.01
W	8	6	.04	.02	.04	.00
X	8	6	.00	.04	.10	.00
W	8	8	.04	.00	.04	.00
X	8	8	.00	.02	.12	.00

Appendix J. Estimated decision error rates for Chen test at the 0.1 level, and Max test, for compositing within sector (DES=W) or across sector (DES=X), based on simulations from Piazza Road Data.

EA = EA # (1 to 7). MEAN and CV denote EA true mean and CV.
M = # of samples per composite. N = # of composite samples.

----------------------------EA=3 MEAN=5.1 CV=1.1----------------------------

DES	M	N	MAX 0.5SSL	MAX 2.0SSL	CHEN 0.5SSL	CHEN 2.0SSL
W	4	4	.01	.03	.03	.01
X	4	4	.00	.11	.14	.00
W	4	6	.02	.00	.00	.00
X	4	6	.00	.03	.11	.00
W	4	8	.06	.00	.00	.00
X	4	8	.00	.01	.10	.00
W	6	4	.00	.02	.01	.00
X	6	4	.00	.09	.12	.00
W	6	6	.01	.00	.00	.00
X	6	6	.00	.03	.11	.00
W	6	8	.02	.00	.00	.00
X	6	8	.00	.01	.11	.00
W	8	4	.00	.02	.01	.00
X	8	4	.00	.10	.14	.00
W	8	6	.01	.00	.00	.00
X	8	6	.00	.03	.12	.00
W	8	8	.03	.00	.00	.00
X	8	8	.00	.01	.12	.00

----------------------------EA=4 MEAN=3.8 CV=1.2----------------------------

DES	M	N	MAX 0.5SSL	MAX 2.0SSL	CHEN 0.5SSL	CHEN 2.0SSL
W	4	4	.01	.11	.07	.00
X	4	4	.00	.11	.10	.00
W	4	6	.02	.04	.06	.00
X	4	6	.00	.04	.11	.00
W	4	8	.02	.01	.05	.00
X	4	8	.00	.01	.09	.00
W	6	4	.01	.10	.05	.00
X	6	4	.00	.10	.12	.00
W	6	6	.00	.02	.04	.00
X	6	6	.00	.03	.09	.00
W	6	8	.01	.01	.04	.00
X	6	8	.00	.02	.10	.00
W	8	4	.00	.09	.04	.00
X	8	4	.00	.12	.12	.00
W	8	6	.00	.03	.06	.00
X	8	6	.00	.03	.11	.00
W	8	8	.00	.01	.03	.00
X	8	8	.00	.01	.11	.00

Appendix J. Estimated decision error rates for Chen test at the 0.1 level, and Max test, for compositing within sector (DES=W) or across sector (DES=X), based on simulations from Piazza Road Data.

EA = EA # (1 to 7). MEAN and CV denote EA true mean and CV.
M = # of samples per composite. N = # of composite samples.

----------------------------EA=5 MEAN=9.3 CV=2.0----------------------------

DES	M	N	MAX 0.5SSL	MAX 2.0SSL	CHEN 0.5SSL	CHEN 2.0SSL
W	4	4	.22	.13	.01	.12
X	4	4	.03	.17	.07	.04
W	4	6	.48	.03	.00	.02
X	4	6	.03	.06	.08	.00
W	4	8	.71	.00	.00	.00
X	4	8	.05	.03	.10	.00
W	6	4	.18	.06	.00	.05
X	6	4	.00	.10	.10	.01
W	6	6	.47	.01	.00	.00
X	6	6	.00	.02	.10	.00
W	6	8	.76	.00	.00	.00
X	6	8	.00	.01	.11	.00
W	8	4	.19	.05	.00	.03
X	8	4	.00	.08	.12	.00
W	8	6	.45	.01	.00	.00
X	8	6	.00	.03	.14	.00
W	8	8	.76	.00	.00	.00
X	8	8	.00	.01	.10	.00

---------------------------EA=6 MEAN=15.8 CV=2.2----------------------------

DES	M	N	MAX 0.5SSL	MAX 2.0SSL	CHEN 0.5SSL	CHEN 2.0SSL
W	4	4	.18	.16	.03	.21
X	4	4	.07	.20	.10	.19
W	4	6	.22	.06	.03	.07
X	4	6	.10	.08	.09	.07
W	4	8	.34	.03	.02	.03
X	4	8	.13	.03	.09	.03
W	6	4	.13	.11	.02	.11
X	6	4	.02	.16	.09	.09
W	6	6	.15	.04	.02	.03
X	6	6	.05	.06	.08	.02
W	6	8	.33	.01	.02	.01
X	6	8	.07	.03	.09	.01
W	8	4	.08	.09	.00	.07
X	8	4	.01	.14	.09	.03
W	8	6	.11	.03	.01	.01
X	8	6	.01	.04	.09	.01
W	8	8	.31	.01	.01	.00
X	8	8	.01	.02	.10	.00

Appendix J. Estimated decision error rates for Chen test at the 0.1 level, and Max test, for compositing within sector (DES=W) or across sector (DES=X), based on simulations from Piazza Road Data.

EA = EA # (1 to 7). MEAN and CV denote EA true mean and CV.
M = # of samples per composite. N = # of composite samples.

-----------------------------EA=7 MEAN=2.8 CV=1.4-----------------------------

DES	M	N	MAX 0.5SSL	MAX 2.0SSL	CHEN 0.5SSL	CHEN 2.0SSL
W	4	4	.03	.11	.02	.00
X	4	4	.00	.13	.09	.00
W	4	6	.09	.03	.02	.00
X	4	6	.01	.06	.07	.00
W	4	8	.16	.01	.02	.00
X	4	8	.01	.02	.09	.00
W	6	4	.02	.08	.01	.00
X	6	4	.00	.10	.12	.00
W	6	6	.06	.02	.01	.00
X	6	6	.00	.03	.09	.00
W	6	8	.10	.00	.01	.00
X	6	8	.00	.02	.09	.00
W	8	4	.01	.06	.01	.00
X	8	4	.00	.10	.12	.00
W	8	6	.04	.01	.00	.00
X	8	6	.00	.03	.10	.00
W	8	8	.06	.00	.00	.00
X	8	8	.00	.01	.11	.00

APPENDIX K

Soil Organic Carbon (K_{oc}) / Water (K_{ow}) Partition Coefficients

Table K-1. Values Used for K_{oc} / K_{ow} Correlation

		Calculated		Measured	
Chemical	log K_{ow}	log K_{oc}	K_{oc}	log K_{oc}	K_{oc} (geomean)
Benzene	2.13	1.77	59	1.79	61.7
Bromoform	2.35	1.94	87	2.10	126
Carbon tetrachloride	2.73	2.24	174	2.18	152
Chlorobenzene	2.86	2.34	219	2.35	224
Chloroform	1.92	1.60	40	1.72	52.5
Dichlorobenzene, 1,2- *(o)*	3.43	2.79	617	2.58	379
Dichlorobenzene, 1,4- *(p)*	3.42	2.79	617	2.79	616
Dichloroethane, 1,1-	1.79	1.50	32	1.73	53.4
Dichloroethane, 1,2-	1.47	1.24	17	1.58	38.0
Dichloroethylene, 1,1-	2.13	1.77	59	1.81	65
Dichloroethylene, *trans* -1,2-	2.07	1.72	52	1.58	38
Dichloropropane, 1,2-	1.97	1.64	44	1.67	47.0
Dieldrin	5.37	4.33	21,380	4.41	25,546
Endosulfan	4.10	3.33	2,138	3.31	2,040
Endrin	5.06	4.09	12,303	4.03	10,811
Ethylbenzene	3.14	2.56	363	2.31	204
Hexachlorobenzene	5.89	4.74	54,954	4.90	80,000
Methyl bromide	1.19	1.02	10	0.95	9.0
Methyl chloride	0.91	0.80	6	0.78	6.0
Methylene chloride	1.25	1.07	12	1.00	10
Pentachlorobenzene	5.26	4.24	17,378	4.51	32,148
Tetrachloroethane, 1,1,2,2-	2.39	1.97	93	1.90	79.0
Tetrachloroethylene	2.67	2.19	155	2.42	265
Toluene	2.75	2.26	182	2.15	140
Trichlorobenzene, 1,2,4-	4.01	3.25	1,778	3.22	1,659
Trichloroethane, 1,1,1-	2.48	2.04	110	2.13	135
Trichloroethane, 1,1,2-	2.05	1.70	50	1.88	75.0
Trichloroethylene	2.71	2.22	166	1.97	94.3
Xylene, *o-*	3.13	2.56	363	2.38	241
Xylene, *m-*	3.20	2.61	407	2.29	196
Xylene, *p-*	3.17	2.59	389	2.49	311

Regression Statistics	
Multiple R	0.9870
R Square	0.9742
Adjusted R Square	0.9733
Standard Error	0.1640
Observations	31

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	29.4358	29.4358	1,094	1.4032E-24
Residual	29	0.7804	0.0269		
Total	30	30.2161			

	Coefficients	*Std. Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	0.0784	0.0748	1.0481	0.3033	-0.0746	0.2314
X Variable 1	0.7919	0.0239	33.0742	0.0000	0.7430	0.8409

Figure K-1. Correlation Plot: log K_{ow} and log K_{oc}

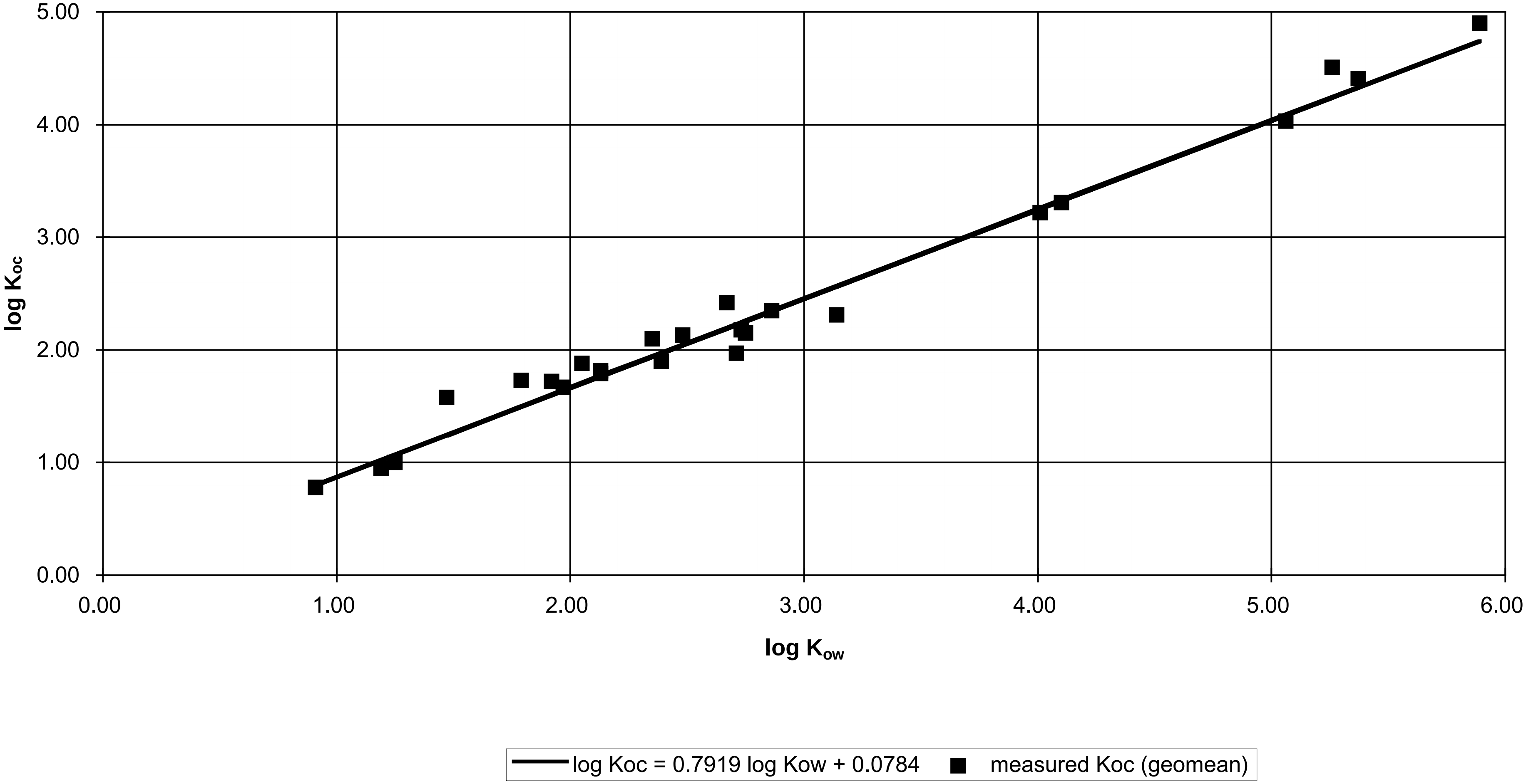


Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Acenaphthene	83-32-9				
		3,890	3.59	Szabo (1990a)	RP-HPLC on PIHAC (humic acids)
		6,166	3.79	Szabo (1990a)	RP-HPLC on CIHAC (humic acids)
Average		***5,028***	3.70		
Geometric Mean		***4,898***	3.69		
Acetone	67-64-1				
Aldrin	309-00-2				
		48,394	4.68	Lord et al. (1980)	"Geescroft/Rothamsted Farm" soil; 2.6% OM; pH=5.1; suspect
		48,978	4.69	Briggs (1981)	Batcombe silt loam (Gr. Br.); 2.05% OC; pH=6.1
Average		***48,686***	4.69		
Geometric Mean		***48,685***	4.69		
Anthracene	120-12-7				
		14,500	4.16	McCarthy & Jimenez (1985)	humic acids
		15,849	4.20	Karichkoff (1981)	soil/sediments average; shake-flask UV
		19,562	4.29	Landrum et al. (1984)	surface water (geomean 5 values)
		23,988	4.38	Hodson & Williams (1988)	cyanopropyl column; HPLC
		26,000	4.41	Karickhoff et al. (1979)	avg. coarse silt fraction, Doe Run & Hickory Hill sediments
		26,303	4.42	Szabo et al. (1990a)	RP-HPLC on PIHAC (humic acids)
		27,840	4.44	Abdul & Gibson (1986)	Flint aquifer sample; 87% sand; foc = 0.0187
		31,329	4.50	Landrum et al. (1984)	humic acid (geomean 8 values)
		33,884	4.53	Szabo et al. (1990a)	RP-HPLC on CIHAC (humic acids)
Average		***24,362***	4.39		
Geometric Mean		***23,493***	4.37		
Benz(α)anthracene	56-55-3				
		150,000	5.18	McCarthy & Jimenez (1985)	humic acid
		199,526	5.30	Landrum et al. (1984)	humic acid
		650,000	5.81	Karickhoff et al. (1979)	avg. coarse silt fraction, Doe Run & Hickory Hill seds.
		840,000	5.92	Smith et al. (1978) as cited in Di Toro et al. (1985)	40% OC
Average		***459,882***	5.66		
Geometric Mean		***357,537***	5.55		
Benzene	71-43-2				
		31	1.50	Chiou et al. (1983)	Woodburn silt loam; fom = 0.019; 21% clay
		38.2	1.58	Seip et al. (1986)	forest soil with 0.2% OC; column study
		43.5	1.64	Seip et al. (1986)	agricultural soil with 2.2% OC; column study
		49	1.69	Abdul et al. (1987)	batch equilibrium experiments; aquifer material; foc = 0.0105
		53.5	1.73	Seip et al. (1986)	forest soil with 3.7% OC; column study
		60	1.78	Karickhoff (1981)	soils/sediments average; shake flask UV

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Benzene	71-43-2				
(continued)		63	1.80	Piwoni & Banerjee (1989)	0.19 percent organic carbon
		66	1.82	Szabo et al. (1990a)	RP-HPLC on PIHAC (humic acids)
		74	1.87	Szabo et al. (1990a)	RP-HPLC on CIHAC (humic acids)
		83	1.92	Karickhoff et al. (1979)	avg. coarse silt fraction, Doe Run & Hickory Hill seds.
		92	1.97	Rogers et al. (1980)	Hastings silty clay loam with 2.6% OC
		98	1.99	Pavlou (1987) as cited in Mackay et al. (1992)	
		100	2.00	Rogers et al. (1980)	Overton silty clay loam with 1.8% OC
Average		***66***	1.82		
Geometric Mean		***62***	1.79		
Benzo(*a*)pyrene	50-32-8				
		478,947	5.68	Smith et al. (1978) as cited in Di Toro (1985)	3.8% OC
		891,251	5.95	Landrum et al. (1984)	humic acids
		2,130,000	6.33	McCarthy & Jimenez (1985)	humic acids (average 8 values)
Average		***1,166,733***	6.07		
Geometric Mean		***968,774***	5.99		
Benzo(*b*)fluoranthene	205-99-2				
Benzo(*k*)fluoranthene	207-08-9				
Bis(2-chlorethyl)ether	111-44-4				
		75.9	1.88	Wilson et al. (1981)	Lincoln sand; 0.087% OC
Average		***76***	1.88		
Geometric Mean		***76***	1.88		
Bis(2-ethylhexyl)phthalate	117-81-7				
(Bis(2-ethylhexyl)ester)		87,420	4.94	Russell & McDuffie (1986)	Broome Co., NY, composite soil; 1.59% OC; column study
		141,254	5.15	Carter & Suffet (1983)	measured change in sorption in presence of humic acids
Average		***114,337***	5.06		
Geometric Mean		***111,123***	5.05		
Bromodichloromethane	75-27-4				
Bromoform	75-25-2				
(Tribromomethane)		126	2.10	Hutzler et al. (1986)	column, Keweenaw 7 soil; 0.85% OC
Average		***126***	2.10		
Geometric Mean		***126***	2.10		

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Butyl benzyl phthalate	85-68-7				
		16,981	4.23	Russell & McDuffie (1986)	Broome County, NY, composite soil with 1.59% OC; column
		11,128	4.05	Gledhill (1980)	3 soils; 1.2-3.4% OC - geomean value calculated from range
Average		***14,055***	4.15		
Geometric Mean		***13,746***	4.14		
Carbazole	86-74-8				
Carbon disulfide	75-15-0				
Carbon tetrachloride	56-23-5				
		123	2.09	Koch (1983)	sorption coefficient (assume Kom) from unpublished source
		127	2.10	Rutherford et al. (1992)	extracted peat; 64% OC
		224	2.35	Abdul et al. (1987)	from MS thesis
Average		***158***	2.20		
Geometric Mean		***152***	2.18		
Chlordane	57-74-9				
		44,711	4.65	Johnson-Logan et al. (1992)	geologic material, N. Hollywood dump (avg. 14 values)
		58,884	4.77	Chin & Weber (1989)	humic acid polymers
Average		***51,798***	4.71		
Geometric Mean		***51,310***	4.71		
Chlorobenzene	108-90-7				
		83	1.92	Chiou et al. (1983)	Woodburn silt loam; fom = 0.019; 21% clay
		117	2.07	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		164	2.22	Schwarzenbach & Westall (1981)	KS1 collected from field site location; foc = 0.0073
		200	2.30	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	system specific information not given
		219	2.34	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	system specific information not given
		260	2.41	Schwarzenbach & Westall (1981)	average of six measurements;foc = 0.0015
		389	2.59	Roberts et al. (1980)	calculated from field data assuming foc = 0.0099
		407	2.61	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	system specific information not given
		500	2.70	Schwarzenbach & Westall (1981)	field sample; 0.08% OC
Average		***260***	2.41		
Geometric Mean		***224***	2.35		
Chlorodibromomethane	124-48-1				
Chloroform	67-66-3				
		28	1.44	Grathwohl (1990)	20 C; soil, sand & loess
		40	1.60	Hutzler et al. (1983)	average of two soils
		76	1.88	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		59	1.77	Loch et al. (1986)	top 20 cm, Eerd soil; 4.06% OC (from unpublished work)

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Chloroform	67-66-3				
(continued)		81	1.91	Loch et al. (1986)	top 20 cm, peat soil ; 11.6% OC (from unpublished work)
Average		***57***	1.75		
Geometric Mean		***53***	1.72		
Chrysene	218-01-9				
DDD	72-54-8				
		45,800	4.66	Gustafson (1989)	average value from collected measured values
Average		***45,800***	4.66		
Geometric Mean		***45,800***	4.66		
DDE	72-55-9				
		86,405	4.94	Koch (1983)	sorption coefficient (assume Kom) from unpublished source
Average		***86,405***	4.94		
Geometric Mean		***86,405***	4.94		
DDT	50-29-3				
		285,467	5.46	Gerstl & Mingelgrin (1984)	Malkiya soil; 5.82% OM
		496,476	5.70	Gerstl & Mingelgrin (1984)	Neve Yaar soil; 2.82% OM
		589,537	5.77	Gerstl & Mingelgrin (1984)	Kinneret G sediment; 4.39% OM
		747,887	5.87	Gerstl & Mingelgrin (1984)	Kinneret A sediment; 7.85% OM
		892,067	5.95	Gerstl & Mingelgrin (1984)	Gilat soil; 1.25% OM
		1,741,516	6.24	Gerstl & Mingelgrin (1984)	Mivtahim soil; 0.45% OM
Average		***792,158***	5.90		
Geometric Mean		***677,934***	5.83		
Dibenz(*a,h*)anthracene	53-70-3				
		565,014	5.75	Means et al. (1980); Hasset et al. (1980)	IL soil; 1.30% OC (EPA-20)
		805,292	5.91	Means et al. (1980); Hasset et al. (1980)	ND sediment; 2.28% OC (EPA-5)
		808,991	5.91	Means et al. (1980); Hasset et al. (1980)	IL sediment; 2.38% OC (EPA-23)
		1,172,847	6.07	Means et al. (1980); Hasset et al. (1980)	IA sediment; 0.15% OC (EPA-8)
		1,690,971	6.23	Means et al. (1980); Hasset et al. (1980)	GA sediment; 1.21% OC (EPA-B2)
		1,687,404	6.23	Means et al. (1980); Hasset et al. (1980)	MO sediment; 2.07% OC (EPA-4)
		2,277,875	6.36	Means et al. (1980); Hasset et al. (1980)	IA loess; 0.11% OC (EPA-9)
		2,383,765	6.38	Means et al. (1980); Hasset et al. (1980)	IL sediment; 1.67% OC (EPA-22)
		2,622,453	6.42	Means et al. (1980); Hasset et al. (1980)	SD sediment; 0.72% OC (EPA-6)
		2,663,317	6.43	Means et al. (1980); Hasset et al. (1980)	IN sediment; 0.95% OC (EPA-15)
		2,691,870	6.43	Means et al. (1980); Hasset et al. (1980)	IL sediment; 1.48% OC (EPA-26)
		2,962,603	6.47	Means et al. (1980); Hasset et al. (1980)	IL sediment; 1.88% OC (EPA-21)
		3,020,262	6.48	Means et al. (1980); Hasset et al. (1980)	WV soil; 0.48% OC (EPA-14)

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Dibenz(*a,h*)anthracene	53-70-3				
(continued)		3,059,425	6.49	Means et al. (1980); Hasset et al. (1980)	KY sediment; 0.66% OC (EPA-18)
Average		***2,029,435***	6.31		
Geometric Mean		***1,789,101***	6.25		
1,2-Dichlorobenzene (*o*)	95-50-1				
		267	2.43	Lee et al. (1989)	untreated Marlette soil, B+ horizon; 0.3% OC
		280	2.45	Lee et al. (1989)	untreated Marlette soil, A horizon; 2.59% OC
		310	2.49	Chiou et al. (1979)	Willamette silt loam; 0.928% OC; 3.5 degrees Celsius
		321	2.51	Chiou et al. (1983)	Woodburn silt loam; 1.9% OM; 9% sand; 68% silt; 21% clay
		386	2.59	Stauffer & MacIntyre (1986)	Appalachee sorbent; 1.4% OC; pH = 6.3
		438	2.64	Stauffer & MacIntyre (1986)	Appalachee sorbent; 1.4% OC; pH = 4.1
		485	2.69	Friesel et al. (1984)	peaty soil; 29% OM
		497	2.70	Piwoni & Banerjee (1989)	sediment, 0.19% OC; avg. 2 values
		529	2.72	Friesel et al. (1984)	foc reported as a range; avg. of several exper.
Average		***390***	2.59		
Geometric Mean		***379***	2.58		
1,4-Dichlorobenzene (*p*)	106-46-7				
		273	2.44	Chiou et al. (1983)	Woodburn silt loam; fom = 0.019; 21% clay
		280	2.45	Southworth & Keller (1986)	Dormont soil with 1.2% OC; 60% clay
		300	2.48	Hutzler et al. (1983)	column; Grayling soil; 1.52% OC; B21 horizon
		398	2.60	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		429	2.63	Friesel et al. (1984)	reported as Kom; foc given as a range
		603	2.78	Schwarzenbach & Westall (1981)	KS1 field sample; 0.73% OC
		665	2.82	Southworth & Keller (1986)	Apison soil with 0.11% OC; 86% clay
		700	2.85	Hutzler et al. (1983)	batch; average of five soils
		724	2.86	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	system specific information not provided
		733	2.87	Schwarzenbach & Westall (1981)	average of six measurements; aquifer material; foc = 0.0015
		832	2.92	Chin & Weber (1989)	humic acid polymers
		850	2.93	Southworth & Keller (1986)	Fullerton soil with 0.06% OC
		911	2.96	Loch et al. (1986)	top 20 cm of Eerd soil; 0.06% OC; column
		1,024	3.01	Wu & Gschwend (1986)	Charles River sediment; 8.5% OC
		1,259	3.10	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	system specific information not provided
		1,375	3.14	Schwarzenbach & Westall (1981)	field sample; 0.08% OC
Average		***687***	2.84		
Geometric Mean		***616***	2.79		
3,3-Dichlorobenzidine	91-94-1				

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
1,1-Dichloroethane	75-34-3				
		46	1.66	Jury et al. (1990)	soil; selected
		62	1.79	Roy et al. (1987)	computed from an isotherm; 4.04% OC
Average		***54***	1.73		
Geometric Mean		***53***	1.73		
1,2-Dichloroethane	107-06-2				
		22	1.34	Jury et al. (1990)	soil; selected
		33	1.52	Chiou et al. (1979)	Willamette silt loam; 0.928% OC; 20 degrees Celsius
		76	1.88	Wilson et al. (1981)	Lincoln sand; 0.087% OC
Average		***44***	1.64		
Geometric Mean		***38***	1.58		
1,1-Dichloroethylene	75-35-4				
		65	1.81	Schwille (1988) (secondary)	
Average		***65***	1.81		
Geometric Mean		***65***	1.81		
***cis* -1,2-Dichloroethylene**	156-59-2				
***trans* -1,2-Dichloroethylene**	156-60-5				
		38	1.58	Brusseau & Rao (1991)	Tampa sandy aquifer material; 0.13% OC; < 2mm
Average		***38***	1.58		
Geometric Mean		***38***	1.58		
1,2-Dichloropropane	78-87-5				
		47	1.67	Chiou et al. (1979)	Willamette silt loam; 0.928% OC; 20 degrees Celsius
Average		***47***	1.67		
Geometric Mean		***47***	1.67		
1,3-Dichloropropene	542-75-6				
		24	1.38	Leistra (1970)	cis- , avg. 3 soils; computed from vapor phase sorption
		26	1.41	Leistra (1970)	trans- , avg. 3 soils; computed from vapor phase sorption
		32	1.51	Wauchope et al. (1992)	trans-, personal comm. (unpublished source, Dow Chemical)
Average		***27***	1.44		
Geometric Mean		***27***	1.43		
Dieldrin	60-57-1				
		23,308	4.37	Sharom et al. (1980)	Beverly sandy loam; 2.5% OM
		26,106	4.42	Sharom et al. (1980)	Plainfield sand; 0.7% OM
		27,399	4.44	Sharom et al. (1980)	Big Creek sediment; 2.8% OM
Average		***25,604***	4.41		
Geometric Mean		***25,546***	4.41		

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Diethyl phthalate	84-66-2				
		69	1.84	Russell & McDuffie (1986)	Broome County, NY, composite soil with 1.59% OC; column
		98	1.99	Russell & McDuffie (1986)	Conklin, NY, sand; 0.26% OC; column; avg. 4 values
Average		***84***	1.92		
Geometric Mean		***82***	1.92		
Dimethyl phthalate	131-11-3				
		7.6	0.88	Seip et al. (1986)	forest soil with 0.2% OC; column study
		42.8	1.63	Seip et al. (1986)	agricultural soil with 2.2% OC; column study
		72.7	1.86	Seip et al. (1986)	forest soil with 3.7% OC; column study
Average		***41***	1.61		
Geometric Mean		***29***	1.46		
Di-*n* -butyl phthalate	84-74-2				
		1,384	3.14	Russell & McDuffie (1986)	Broome County, NY, composite soil with 1.59% OC; column
		1,775	3.25	Russell & McDuffie (1986)	Conklin, NY, sand; 0.26% OC; adsorp.; avg. 4 values; column
Average		***1,580***	3.20		
Geometric Mean		***1,567***	3.20		
2,4-Dinitrotoluene	121-14-2				
2,6-Dinitrotoluene	606-20-2				
Di-*n* -octyl phthalate	117-84-0				
Endosulfan	115-29-7				
		2,040	3.31	Gustafson (1989)	average value from collected measured values
Average		***2,040***	3.31		
Geometric Mean		***2,040***	3.31		
Endrin	72-20-8				
		7,724	3.89	Sharom et al. (1980)	Beverly sandy loam; 2.5% OM
		7,793	3.89	Sharom et al. (1980)	organic soil; 75.3% OM
		14,285	4.15	Sharom et al. (1980)	Plainfield sand; 0.7% OM
		15,885	4.20	Sharom et al. (1980)	Big Creek sediment; 2.8% OM
Average		***11,422***	4.06		
Geometric Mean		***10,811***	4.03		
Ethylbenzene	100-41-4				
		165	2.22	Chiou et al. (1983)	Woodburn silt loam; fom = 0.019; 21% clay
		184	2.27	Lee et al. (1989)	untreated St. Clair soil; 0.44% OC; 44% clay; B+ horizon
		191	2.28	Lee et al. (1989)	untreated Oshtemo soil; 0.11% OC; 6.3% clay; B+ horizon
		240	2.38	Hodson & Williams (1988)	HPLC; cyanopropyl column

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Ethylbenzene	100-41-4				
(continued)		255	2.41	Vowles & Mantoura (1987)	Tamar estuary sediment; 4.02% OC; 0.2% synth. sea salt
Average		***207***	2.32		
Geometric Mean		***204***	2.31		
Fluoranthene	206-44-0				
		41,687	4.62	Szabo et al. (1990a)	RP & HPLC on PIHAC (humic acids)
		51,658	4.71	Abdul & Gibson (1986)	Flint aquifer sample; 87% sand; foc = 0.0187
		54,954	4.74	Szabo et al. (1990a)	RP & HPLC on CIHAC (humic acids)
Average		***49,433***	4.69		
Geometric Mean		***49,096***	4.69		
Fluorene	86-73-7				
		3,989	3.60	Abdul et al. (1986)	Borden aquifer material (avg. 2 values, foc = 0.0091,0.0121)
		4,615	3.66	Abdul et al. (1986)	Flint aquifer material (avg. 8 values)
		5,576	3.75	Abdul et al. (1986)	Warren aquifer material (avg. 8 values)
		8,913	3.95	Carter & Suffet (1983)	humic materials (DOC)
		14,125	4.15	Szabo et al. (1990a)	RP-HPLC on CIHAC (humic acids)
		16,218	4.21	Szabo et al. (1990a)	RP-HPLC on PIHAC (humic acids)
Average		***8,906***	3.95		
Geometric Mean		***7,707***	3.89		
Heptachlor	76-44-8				
		6,810	3.83	Jury et al. (1990)	selected
		13,330	4.12	Gustafson (1989)	average value from collected measured values
Average		***10,070***	4.00		
Geometric Mean		***9,528***	3.98		
Heptachlor epoxide	1024-57-3				
Hexachlorobenzene	118-74-1				
		80,000	4.90	Karickhoff & Morris (1985a)	GA sediments; 0.5-1.5% OC
Average		***80,000***	4.90		
Geometric Mean		***80,000***	4.90		
Hexachloro-1,3-butadiene	87-68-3				
α-Hexachlorocyclohexane	319-84-6				
(alpha-BHC)		1,022	3.01	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.62% OM
		1,253	3.10	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.27% OM
		1,330	3.12	Wahid & Sethunathan (1979)	single measurement; Kari soil; 24.6% OM
		1,386	3.14	Wahid & Sethunathan (1979)	single measurement; sandy soil; 12.6% OM
		1,532	3.19	Wahid & Sethunathan (1979)	single measurement; alluvial soil; 0.75% OM

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
α-Hexachlorocyclohexane	319-84-6				
(continued)		2,004	3.30	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 2.88% OM
		2,024	3.31	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.00% OM
		2,090	3.32	Wahid & Sethunathan (1979)	single measurement; Pokkali soil; 5.52% OM
		2,123	3.33	Wahid & Sethunathan (1979)	single measurement; Kari soil; 8.21% OM
		2,168	3.34	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 0.60% OM
		2,200	3.34	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 0.92% OM
		2,891	3.46	Wahid & Sethunathan (1979)	single measurement; alluvial soil; 0.70% OM
Average		***1,835***	3.26		
Geometric Mean		***1,762***	3.25		
β-Hexachlorocyclohexane	319-85-7				
(beta-BHC)		1,156	3.06	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.27% OM
		1,470	3.17	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.62% OM
		1,681	3.23	Wahid & Sethunathan (1979)	single measurement; Kari soil; 24.6% OM
		1,794	3.25	Mills & Biggar (1969b)	Venado clay; 3.5% OC; 50% montmorillonite; 20° C; 1/n=0.861
		1,821	3.26	Wahid & Sethunathan (1979)	single measurement; sandy soil; 12.6% OM
		1,868	3.27	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.00% OM
		1,958	3.29	Wahid & Sethunathan (1979)	single measurement; alluvial soil; 0.75% OM
		2,098	3.32	Wahid & Sethunathan (1979)	single measurement; alluvial soil; 0.70% OM
		2,415	3.38	Wahid & Sethunathan (1979)	single measurement; Kari soil; 8.21% OM
		2,548	3.41	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 0.60% OM
		2,697	3.43	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 0.92% OM
		3,143	3.50	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 2.88% OM
		3,158	3.50	Wahid & Sethunathan (1979)	single measurement; Pokkali soil; 5.52% OM
		3,563	3.55	Mills & Biggar (1969b)	Staten peaty muck, 12.8% OC; 20° C; 1/n = 0.950
Average		***2,241***	3.35		
Geometric Mean		***2,139***	3.33		
γ-Hexachlorocyclohexane	58-89-9				
(Lindane)		731	2.86	Adams & Li (1971)	Svea sil, A horizon ; foc = 0.031
		735	2.87	McCall et al. (1980)	average for three soils, 0.68-2.01% OC
		757	2.88	Huggenberger et al. (1972)	Gila silt loam; foc = 0.0038; coulmn study
		760	2.88	Kishi et al. (1990)	clay loam (allophane); soil pH = 4.89; foc = 0.104
		760	2.88	Wahid & Sethunathan (1980)	latertic soil; 2.88% OM; 1:1
		764	2.88	Adams & Li (1971)	Hegne sic, A horizon ; foc = 0.043
		764	2.88	Adams & Li (1971)	Hegne sic, B horizon ; foc = 0.006
		769	2.89	Adams & Li (1971)	Fargo sic, A horizon ; foc = 0.052
		812	2.91	Adams & Li (1971)	Hubbard ls, A horizon ; foc = 0.012
		814	2.91	Adams & Li (1971)	Ontonagon c, A horizon ; foc = 0.035
		826	2.92	Adams & Li (1971)	Milaca sl, A horizon ; foc = 0.017
		852	2.93	Mills & Biggar (1969a)	1.1% OC; Ca Columbia silt loam

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
γ-Hexachlorocyclohexane	58-89-9				
(continued)		855	2.93	Adams & Li (1971)	Kranzburg sicl, B horizon ; foc = 0.01
		878	2.94	Adams & Li (1971)	Svea sil, B horizon ; foc = 0.008
		960	2.98	Kishi et al. (1990)	sandy loam (allophane); soil pH = 5.41; foc = 0.0791
		968	2.99	Kay & Elrick (1967)	Muck (38% OC)
		985	2.99	Adams & Li (1971)	Fayette sil, A horizon ; foc = 0.023
		986	2.99	Kay & Elrick (1967)	Honeywood loam (2.1% OC)
		1,005	3.00	Adams & Li (1971)	Canisteo cl, B horizon ; foc = 0.006
		1,010	3.00	Rippen et al. (1982)	Alfisol; Udalf, Para brown earth; 0.76% OC; soil pH = 7.45
		1,030	3.01	Kay & Elrick (1967)	Fox loamy sand (1.7% OC)
		1,079	3.03	Adams & Li (1971)	Lester fsl, A horizon ; foc = 0.023
		1,103	3.04	Huggenberger et al. (1972)	Pachappa sandy loam; foc = 0.005
		1,103	3.04	Sharom et al. (1980)	Beverly sand loam; 2.5% OM
		1,109	3.04	Wahid & Sethunathan (1979)	single measurement; sandy soil; 12.6% OC
		1,125	3.05	Adams & Li (1971)	Zimmerman s, A horizon ; foc = 0.007
		1,130	3.05	Huggenberger et al. (1972)	Kentwood sandy loam; foc = 0.0093
		1,200	3.08	Kishi et al. (1990)	light clay (montmorillonite - illite); pH = 5.26; foc = 0.0323
		1,204	3.08	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.27% OM
		1,227	3.09	Kay & Elrick (1967)	Brookstone sandy loam (1.9% OC)
		1,263	3.10	Adams & Li (1971)	Brainerd fsl, A horizon ; foc = 0.026
		1,274	3.11	Adams & Li (1971)	Bearden sil, B horizon ; foc = 0.002
		1,300	3.11	Kishi et al. (1990)	light clay (montmorillonite); soil pH = 5.18; foc = 0.0151
		1,300	3.11	McCall et al. (1983)	Not stated if these are original data
		1,318	3.12	Miller & Weber (1986)	Ann Arbor soil; 1.14% OC
		1,322	3.12	Moreale & van Bladel (1978)	Lubbeek II soil; 0.53% OC; 10% clay
		1,335	3.13	Moreale & van Bladel (1978)	Lubbeek I soil; 0.07% OC; 2% clay
		1,452	3.16	Mills & Biggar (1969a)	3.1% OC; Ca Venado clay
		1,455	3.16	Adams & Li (1971)	Brainerd sl, B horizon ; foc = 0.001
		1,458	3.16	Miller & Weber (1986)	Delta soil; 0.12% TOC
		1,478	3.17	Sharom et al. (1980)	Big Creek sediment; 2.8% OM
		1,525	3.18	Wahid & Sethunathan (1978)	Pokkali soil; 5.52% OM; 1:10; 5 min eq.
		1,580	3.20	Wahid & Sethunathan (1980)	Pokkali soil; 5.52% OM; 1:1
		1,681	3.23	Wahid & Sethunathan (1979)	single measurement; Kari soil; 24.6% OM
		1,724	3.24	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.00% OM
		1,830	3.26	Adams & Li (1971)	Blue Earth sil, A horizon ; foc = 0.11
		1,859	3.27	Caron et al. (1985)	Powerville sediment (NJ); 2-4% OC
		1,896	3.28	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 2.88% OM
		1,935	3.29	Wahid & Sethunathan (1979)	single measurement; alluvial soil; 0.70% OM
		1,970	3.29	Sharom et al. (1980)	Plainfield sand; 0.7% OM
		1,976	3.30	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 1.62% OM
		2,058	3.31	Sharom et al. (1980)	organic soil; 75.3% OM
		2,090	3.32	Wahid & Sethunathan (1979)	single measurement; Pokkali soil; 5.52% OM
		2,122	3.33	Wahid & Sethunathan (1979)	single measurement; alluvial soil; 0.75% OM

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
γ-Hexachlorocyclohexane	58-89-9				
(continued)		2,123	3.33	Wahid & Sethunathan (1979)	single measurement; Kari soil; 8.21% OM
		2,260	3.35	Spencer & Cliath (1970)	Gila silt loam; 0.35% OC; from vapor phase desorp.; 30° C
		2,268	3.36	Adams & Li (1971)	Blue Earth sil, B horizon ; foc = 0.083
		2,290	3.36	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 0.92% OM
		2,448	3.39	Wahid & Sethunathan (1979)	single measurement; lateritic soil; 0.60% OM
		2,584	3.41	Mills & Biggar (1969a)	11.9% OC; Staten peaty muck
		2,646	3.42	Miller & Weber (1986)	Michaywe soil; 0.13% TOC
		2,710	3.43	Moreale & van Bladel (1978)	Zolder soil; 0.19% OC; 1% clay
		2,926	3.47	Wahid & Sethunathan (1978)	alluvial soil; 0.75% OM; 1:20; 5 min equlibration
		2,983	3.47	Chiou et al. (1979)	Willamette silt loam; 1.6% OM; 26% clay
		3,249	3.51	Adams & Li (1971)	Ulen sl, B horizon ; foc = 0.003
Average		***1,477***	3.17		
Geometric Mean		***1,352***	3.13		
Hexachlorocyclopentadiene	77-47-4				
Hexachloroethane	67-72-1				
Indeno(1,2,3-*cd*)pyrene	193-39-5				
Isophorone	78-59-1				
(Isooctaphenone)					
Methoxychlor	72-43-5				
		80,000	4.90	Karickhoff et al. (1979)	avg. Doe Run and Hickory Hill coarse silt sed. fractions
Average		***80,000***	4.90		
Geometric Mean		***80,000***	4.90		
Methyl bromide	74-83-9				
(Bromomethane)		9	0.95	Briggs (1981)	presented as a value for several chemicals
Average		***9***	0.95		
Geometric Mean		***9***	0.95		
Methyl chloride	75-09-2				
(chloromethane)		6	0.78	Jury et al. (1990)	soil; selected
Average		***6***	0.78		
Geometric Mean		***6***	0.78		
Methylene chloride	75-09-2				
(Dichloromethane)		10	1.00	Daniels et al. (1985)	selected
Average		***10***	1.00		
Geometric Mean		***10***	1.00		

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Naphthalene	91-20-3				
		830	2.92	Kishi et al. (1990)	light clay; 1.51% OC
		843	2.93	Vowles & Mantoura (1987)	Tamar estuary sediment; 4.02% OC; 0.2% synth. sea salt
		871	2.94	Karickhoff (1981)	soils/sediments average; shake flask UV
		907	2.96	Stauffer & MacIntyre (1986)	Appalachee soil; 1.4% OC; pH = 3.1
		912	2.96	Hodson & Williams (1988)	unpublished experimental results by same authors
		960	2.98	Southworth & Keller (1986)	Fullerton soil; 0.06% OC
		1,000	3.00	Southworth & Keller (1986)	Apison soil; 0.11% OC
		1,000	3.00	Kan & Tomson (1990)	DOM
		1,096	3.04	McCarthy & Jiminez (1985)	humic acid polymers
		1,161	3.06	Lokke (1984)	avg. 10 values
		1,290	3.11	Rippen et al. (1982)	Alfisol; 0.76% OC
		1,300	3.11	Karickhoff et al. (1979)	average of Doe Run & Hickory Hill sediments
		1,333	3.12	Karickhoff (1982)	Mississippi River sediment; foc = 0.015
		1,400	3.15	Podoll et al. (1989)	Menlo Park soil; 1.6% OC
		1,413	3.15	Szabo et al. (1990a)	RP-HPLC on CIHAC (humic acids)
		1,440	3.16	Rippen et al. (1982)	Entisol; 1.11% OC
		1,445	3.16	Szabo et al. (1990a)	RP-HPLC on PIHAC (humic acids)
		1,610	3.21	Rippen et al. (1982)	Speyer soil, 0.15-0.5 mm; 1.12% OC
		1,861	3.27	Barrett et al. (1994)	soil; 0.13% OC
		1,950	3.29	Wood et al. (1990)	Eustis sand; 0.74% OC; batch & column data
Average		***1,231***	3.09		
Geometric Mean		***1,191***	3.08		
Nitrobenzene	98-95-3				
		30.6	1.49	Seip et al. (1986)	forest soil with 0.2% OC; column study
		76	1.88	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		86	1.93	Briggs (1981)	average for four soils; 0.6-2.5% OC
		88.8	1.95	Seip et al. (1986)	agricultural soil with 2.2% OC; column study
		103	2.01	Seip et al. (1986)	forest soil with 3.7% OC; column study
		142	2.15	Miller & Weber (1986)	Delta soil with foc = 0.0012
		190	2.28	Lokke (1984)	Gribskov B horizon soil; 2.58%OC; avg. 2 values
		191	2.28	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		229	2.36	Hodson & Williams (1988)	unpublished experimental results by same authors
		270	2.43	Lokke (1984)	Gribskov C horizon soil; 1.82%OC; avg. 2 values
Average		***141***	2.15		
Geometric Mean		***119***	2.08		
Pentachlorobenzene	608-93-5				
		11,381	4.06	Wu & Gschwend (1986)	Iowa soil; 2.1% OC
		35,455	4.55	Wu & Gschwend (1986)	North River sediments; approx. 4.4% OC
		38,560	4.59	Barber et al. (1992)	sand/gravel aquifer; avg, 2 measurements; 0.054, 0.062% OC
		40,000	4.60	Karickhoff & Morris (1985a)	GA sediments; 0.5-1.5% OC

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Pentachlorobenzene	608-93-5				
(continued)		55,176	4.74	Wu & Gschwend (1986)	Charles River sediments; approx. 8.5% OC
Average		***36,114***	4.56		
Geometric Mean		***32,148***	4.51		
Pyrene	129-00-0				
		43,807	4.64	Means et al. (1980)	IL sediment with 2.38% OC (EPA-23)
		45,709	4.66	Abdul et al. (1987)	aquifer material, 1.05% OC
		48,236	4.68	Means et al. (1980)	IL sediment with 1.67% OC (EPA-22)
		50,650	4.70	Means et al. (1980)	ND sediment with 2.28% OC (EPA-5)
		51,469	4.71	Means et al. (1980)	ND sediment with 2.07% OC (EPA-4)
		54,767	4.74	Woodburn et al. (1989)	Webster soil; 2.23% OC; 14 C; 30:70 methanol:water
		57,763	4.76	Means et al. (1980)	WV soil with 0.48% OC (EPA-14)
		58,884	4.77	Szabo et al. (1990a)	RP-HPLC on PIHAC (humic acids)
		59,515	4.77	Means et al. (1980)	IL sediment with 1.88% OC (EPA-21)
		59,646	4.78	Means et al. (1980)	IL soil with 1.30% OC (EPA-20)
		61,936	4.79	Abdul & Gibson (1986)	Flint aquifer sample; 87% sand; foc = 0.0187
		62,860	4.80	Means et al. (1980)	GA sediment with 1.21% OC (EPA-B2)
		63,400	4.80	Hassett et al. (1980)	from regression of 14 sediments/soil samples
		64,706	4.81	Means et al. (1980)	IA loess with 0.11% OC (EPA-9)
		66,069	4.82	Szabo et al. (1990a)	RP-HPLC on CIHAC (humic acids)
		67,189	4.83	Means et al. (1980)	IL sediment with 1.48% OC (EPA-26)
		67,467	4.83	Means et al. (1980)	IA sediment with 0.15% OC (EPA-8)
		67,608	4.83	Karickhoff (1981)	soils/sediments average
		76,316	4.88	Means et al. (1980)	KY sediment with 0.66% OC (EPA-18)
		82,421	4.92	Means et al. (1980)	IN sediment with 0.95% OC (EPA-15)
		84,000	4.92	Karickhoff et al. (1979)	avg. Doe Run, Hickory Hill coarse silt sediment fractions
		84,000	4.92	Karickhoff (1982)	Mississippi R. sediment, 1.5% OC
		85,256	4.93	Means et al. (1980)	SD sediment with 0.72% OC (EPA-6)
		87,833	4.94	Karickhoff & Morris (1985b)	Mississippi R. sediment, 1.48% OC (desorption)
		95,395	4.98	Karickhoff & Morris (1985b)	Ohio R. sediment; 3.04% OC (desorption)
		131,325	5.12	Gauthier et al. (1986)	fluoresc. quench. tech.; 13 soil humic & fulvic acids (avg.)
		133,590	5.13	Vowles & Mantoura (1987)	Tamar estuary sediment; 4.02% OC; 0.2% synth. sea salt
Average		***70,808***	4.85		
Geometric Mean		***67,992***	4.83		
Stryene	100-42-5				
		912	2.96	Bedient et al. (1983) as cited in Meylan et al. (1992)	experimental measurement
Average		***912***	2.96		
Geometric Mean		***912***	2.96		

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
1,1,2,2-Tetrachloroethane	79-34-5				
		79	1.90	Chiou et al. (1979)	Willamette silt loam; 0.928% OC; 20 degrees Celsius
Average		***79***	1.90		
Geometric Mean		***79***	1.90		
Tetrachloroethylene	127-18-4				
		177	2.25	Seip et al. (1986)	forest soil with 0.2% OC; column stufy
		205	2.31	Seip et al. (1986)	agricultural soil wtih 2.2% OC; column study
		224	2.35	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	specific system information not provided
		224	2.35	Piwoni & Banerjee (1989)	n-core sediment; foc = 0.0133
		225	2.35	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		235	2.37	Piwoni & Banerjee (1989)	avg. 8 values; J-core sed.; foc = 0.0015 - 0.0089; avg. 1/n>0.94
		237	2.38	Friesel et al. (1984)	reported as Ksom; foc reported as a range; 32 soils
		263	2.42	Abdul et al. (1987)	equilibrium batch experiments; aquifer material; foc = 0.0105
		268	2.43	Pignatello (1990)	Agawam fine sandy loam soil; 2.57% OC; avg. 2 values
		269	2.43	Brusseau & Rao (1991)	Tampa sandy aquifer material; 0.13% OC; < 2mm
		311	2.49	Loch et al. (1986)	top 20 cm of Podzol soil; 0.87% OC
		348	2.54	Seip et al. (1986)	forest soil with 3.7% OC; column study
		356	2.55	Paviostathis & Mathavan (1992)	coarse sand with 0.09% OC
		362	2.56	Chiou et al. (1979)	Willamette silt loam; 0.93% OC; 20 degrees Celsius
		373	2.57	Schwarzenbach & Westall (1981)	avg. of 6 meas. w/ different Co & sorbents; 0.15% OC
Average		***272***	2.43		
Geometric Mean		***265***	2.42		
Toluene	108-88-3				
		94.4	1.97	Seip et al. (1986)	agricultural soil wtih 2.2% OC; column study
		99	2.00	Vowles & Mantoura (1987)	Tamar estuary sediment; 4.02% OC; 0.2% synth. sea salt
		115	2.06	Abdul et al. (1987)	equilibrium batch experiments, aquifer material; foc = 0.0105
		123	2.09	Garbarini & Lion (1986)	zein; 57% OC
		126	2.10	Szabo et al. (1990a)	RP-HPLC on PIHAC (avg., humic acids)
		134	2.13	Seip et al. (1986)	forest soil with 3.7% OC; column study
		150	2.18	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		151	2.18	Garbarini & Lion (1986)	Sapsucker Woods soil with 7.51%C
		151	2.18	Garbarini & Lion (1986)	lignin; 65% OC
		164	2.21	Garbarini & Lion (1986)	Sapsucker Woods ether extracted soil with 7.05%C
		182	2.26	Szabo et al. (1990a)	RP-HPLC on CIHAC (avg., humic acids)
		247	2.39	Schwarzenbach & Westall (1981)	avg. of 6 meas. w/ different Co & sorbents; 0.15% OC
Average		***145***	2.16		
Geometric Mean		***140***	2.15		

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Toxaphene	8001-35-2				
		95,816	4.98	Gustafson (1989)	average value from collected measured values
Average		***95,816***	4.98		
Geometric Mean		***95,816***	4.98		
1,2,4-Trichlorobenzene	120-82-1				
		864	2.94	Chiou et al. (1983)	Woodburn silt loam; fom = 0.019; 21% clay
		885	2.95	Southworth & Keller (1986)	Dormont soil; 1.2% OC
		1,033	3.01	Scheunert et al. (1994)	soil; 2.06% OC
		1,300	3.11	Southworth & Keller (1986)	Fullerton soil; 0.06% OC
		1,303	3.11	Banerjee et al. (1985)	average of 21 values; subsurface alluvial soil
		1,389	3.14	Wilson et al. (1981)	average of two values
		1,435	3.16	Friesel et al. (1984)	peaty soil; 0.29% OM
		1,441	3.16	Friesel et al. (1984)	reported as Ksom; foc reported as a range
		1,554	3.19	Lee et al. (1989)	untreated Marlette soil, A horizon; 2.59% OC
		1,867	3.27	Lee et al. (1989)	untreated Marlette soil, Bt horizon; 0.3% OC
		1,986	3.30	Schwarzenbach & Westall (1981)	KS1 field material; foc = 0.0073
		1,995	3.30	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	system specific information not provided
		2,100	3.32	Southworth & Keller (1986)	Apison soil with 0.11% OC
		2,347	3.37	Schwarzenbach & Westall (1981)	avg. of 6 meas. w/ different Co & sorbents; 0.15% OC
		2,570	3.41	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	system specific information not provided
		3,118	3.49	Wu & Gschwend (1986)	Charles River sediment with approximately 8.8% OC
		3,125	3.49	Schwarzenbach & Westall (1981)	field sample; 0.8% OC
Average		***1,783***	3.25		
Geometric Mean		***1,659***	3.22		
1,1,1-Trichloroethane	71-55-6				
		105.9	2.02	Loch et al. (1986)	top 20 cm of Eerd soil; 4% OC
		107	2.03	Friesel et al. (1984)	reported as Ksom; foc reported as a range
		129	2.11	Hodson & Williams (1988)	cyanopropyl column, HPLC
		172	2.24	Loch et al. (1986)	top 20 cm of Podzol soil; 0.87% OC
		179	2.25	Chiou et al. (1979)	Willamette silt loam; 0.93% OC; 3.5 degrees Celsius
Average		***139***	2.14		
Geometric Mean		***135***	2.13		
1,1,2-Trichloroethane	79-00-5				
		60.0	1.78	Seip et al. (1986)	forest soil with 0.2% OC; column study
		63.7	1.80	Seip et al. (1986)	agricultural soil wtih 2.2% OC; column study
		76	1.88	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		108	2.03	Seip et al. (1986)	forest soil with 3.7% OC; column study
Average		***77***	1.89		
Geometric Mean		***75***	1.87		

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
Trichloroethylene	79-01-6				
		57	1.76	Rutherford & Chiou (1992)	peat; 57% OC
		63	1.80	Smith et al. (1990)	soil; 4.02% OC (from vapor phase experiments)
		65	1.81	Abdul et al. (1987)	equilibrium batch experiments; aquifer material; foc = 0.0105
		69	1.84	Brusseau & Rao (1991)	Tampa sandy aquifer material; 0.13% OC; < 2mm
		72.5	1.86	Seip et al. (1986)	forest soil with 0.2% OC; column study
		84	1.92	Stauffer & MacIntyre (1986)	Appalachee soil; 1.4% OC; pH = 3.2
		84	1.93	Piwoni & Banerjee (1989)	aquifer solid; 0.19% OC
		87	1.94	Rogers & McFarlane (1981)	Overton silty clay loam; foc=0.018; 1/n=0.93
		92	1.96	Wilson et al. (1981)	Lincoln sand; 0.087% OC
		95.8	1.98	Seip et al. (1986)	agricultural soil wtih 2.2% OC; column study
		99	2.00	Pignatello (1990a)	Agawam soil; 2.57% OC (2 values)
		100	2.00	Doust & Huang (1992) as cited in Mackay et al. (1993)	organic carbon soil
		101	2.00	Friesel et al. (1984)	reported as Kom; foc reported as a range; 32 soils
		103	2.01	Loch et al. (1986)	top 20 cm of Eerd soil; 4% OC
		106	2.03	Garbarini & Lion (1986)	Sapsucker Woods soil with 7.51%C
		111	2.05	Garbarini & Lion (1986)	zein; 57% OC
		120	2.08	Garbarini & Lion (1986)	lignin; 65% OC
		122	2.09	Garbarini & Lion (1986)	sapsucker woods ether extracted soil; 7.05% OC
		123	2.09	Hutzler et al. (1986)	column; Keweenaw 7 soil; 0.85% OC (avg. 3 values)
		142	2.15	Seip et al. (1986)	forest soil with 3.7% OC; column study
		150	2.17	Rogers & McFarlane (1981)	Hastings silty clay loam; foc = 0.026; Freundlich; 1/n = 0.82
Average		***97***	1.99		
Geometric Mean		***94***	1.97		
Vinyl chloride	75-01-4				
***o* -Xylene**	95-47-6				
		222	2.35	Vowles & Mantoura (1987)	Tamar estuary sediment; 4.02% OC; 0.2% synth. sea salt
		234	2.37	Szabo et al. (1990a)	RP-HPLC, CIHAC (humic acids)
		251	2.40	Szabo et al. (1990a)	RP-HPLC, PIHAC (humic acids)
		258	2.41	Roy et al. (1987)	Catlin sorbent at 23 degrees Celsius; 4.04% OC
Average		***241***	2.38		
Geometric Mean		***241***	2.38		
***m* -Xylene**	108-38-3				
		158	2.20	Seip et al. (1986)	agricultural soil with 2.2% OC; column study
		166	2.22	Abdul et al. (1987)	equilibrium batch experiments; aquifer material; foc = 0.0105
		289	2.46	Seip et al. (1986)	forest soil; 3.7% OC; column study
Average		***204***	2.31		
Geometric Mean		***196***	2.29		

Table K-2. Collected K_{oc} Values (Hydrophobic Organics)

Chemical	CAS No.	K_{oc} (L/kg)	Log K_{oc}	Source	Comments
***p* -Xylene**	106-42-3				
		260	2.41	Vowles & Mantoura (1987)	Tamar estuary sed.; 4.02% OC; 0.2% synthetic sea salt
		333	2.52	Schwarzenbach & Westall (1984)	soil; 0.15% OC; avg. 6 values
		347	2.54	Schwarzenbach & Giger (1982) as cited in Gerstl (1990)	system specific information not provided
Average		***313***	2.50		
Geometric Mean		***311***	2.49		

Soil/Water Partition Coefficient (K_{oc}) Bibliography

Abdul, A.S., and T.L. Gibson. 1986. Equilibrium batch experiments with six polycyclic aromatic hydrocarbons and two aquifer materials. *Hazardous Waste & Hazardous Materials* 3(2):125-137.

Abdul, A.S., T.L. Gibson and D.N. Rai. 1986. The effect of organic carbon on the adsorption of fluorene by aquifer materials. *Hazardous Waste & Hazardous Materials* 3(4):429-440.

Abdul, A.S., T.L. Gibson, and D.N. Rai. 1987. Statistical correlations for predicting the partition coefficient for nonpolar organic contaminants between aquifer organic carbon and water. *Hazardous Waste & Hazardous Materials* 4(3):211-222.

Adams, R. S., and P. Li. 1971. Soil properties influencing sorption and desorption of lindane. *Soil Science Society of America Proceedings*. 35:78-81.

Banerjee, P., M.D. Piwoni, and K. Ebeid. 1985. Sorption of organic contaminants to a low carbon subsurface core. *Chemosphere*. 14(8):1057-1067.

Barber, L.B., II, E.M. Thurman, and D.D. Runnells. 1992. Geochemical heterogeneity in a sand and gravel aquifer: Effect of sediment mineralogy and particle size on the sorption of chlorobenzen. *J. Cont. Hydrol*. 9:35-54.

Barrett, M.H.,D.J. Williamson, and D.N. Lerner. 1994. A continuous flow method for calculating adsorption isotherms of organic pollutants onto aquifer materials. *J. Cont. Hydrol*. 15:15-25.

Briggs, G.G. 1981. Theoretical and experimental relationships betwen soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors and the parachor. *J. Agric. Food Chem.* 29(5):1050-1059.

Brusseau, M.L., and P.S.C. Rao. 1991. Influence of sorbent structure on nonequilibrium sorption of organic compounds. *Environ. Sci. Technol.* 25(8):1501-1506.

Caron, G., I.H. Suffet, and T. Belton. 1985. Effect of dissolved organic carbon on the environmental distribution of nonpolar organic compounds.*Chemosphere*.14(8):993-1000.

Carter, C.W., and I.H. Suffet. 1983. Interactions between disolved humic and fulvic acids and pollutants in aquatic environments. *Fate of Chemicals in the Environment.* R. L. Swann and A. Eschenroeder, eds. ACS Symposium Series 225. American Chemical Society, Washington, DC. 215-229.

Chin, Y.P, and W.J. Weber, Jr. 1989. Estimating the effects of dispersed organic polymers on the sorption of contaminants by natural solids. 1. A predictive thermodynamic humic substance-organic solute interaction model. *Environ. Sci. Technol.* 23(8):978-984.

Chiou, C.T., L.J. Peters, and V.H. Freed. 1979. A physical concept of soil-water equilibria for nonionic organic compounds. *Science.* 206:831-832.

Chiou, C.T., P.E. Porter, and D.W. Schmedding. 1983. Partition equilibria of nonionic organic compounds between soil organic matter and water. *Environ. Sci. Technol.* 17(4):227-231.

Daniels, S. L., F. D. Hoerger, and R. J. Moolenar. 1985. Environmental exposure assessment: experience under the Toxics Substance Control Act. *Environ. Toxicol. Chem*. 4:107-117.

Di Toro, D.M. 1985. A particle interaction model of reversible organic chemical sorption. *Chemosphere.* 14(10):1503-1538.

Friesel, P., G. Milde, and B. Steiner. 1984. Interactions of halogenated hydrocarbons with soils. *Fresenius Z. Anal. Chem.* 319:160-164.

Garbarini, D.R., and L.W. Lion. 1986. Influence of the nature of soil organics on the sorption of toluene and trichloroethylene. *Environ. Sci. Technol.* 20(12):1263-1269.

Gauthier, T.D., W.R. Seltz, and C.L. Grant. 1987. Effects of structural and compositional variations of dissolved humic materials on pyrene K_{oc} values. *Environ. Sci. Technol.* 21(3):243-248.

Gerstl, Z. 1990. *Evaluating the Groundwater Pollution Hazard of Toxic Organics by Molecular Connectivity*. Final Report. Institute of Soils and Water, The Volcani Center, Bet Dagan, Israel.

Gerstl, Z., and U. Mingelgrin. 1984. Sorption of organic substances by soils and sediments. *J. Environ. Sci. Health* B19(3):297-312.

Gledhill, W.E., R.G. Kaley, W.J. Adams, O. Hicks, P. R. Michael, V.W. Saeger, and G. A. LeBlanc. 1980. An environmental safety assessment of butyl benzyl phthalate. *Environ. Sci. Technol.* 14(3):301-305.

Grathwohl, P. 1990. Influence of organic matter from soils and sediments from various origins on the sorption of some chlorinated aliphatic hydrocarbons: implications on K_{oc} correlations. *Environ. Sci. Technol.* 24(11):1687-1693.

Hassett, J.J., J.C. Means, W.L. Banwart, and S.G. Wood. 1980. *Sorption Properties of Sediments and Energy-Related Pollutants.* EPA 600/3-80-041. U.S. Environmental Protection Agency. Athens, GA.

Hodson, J., and N.A. Williams. 1988. The estimation of the adsorption coefficient (K_{oc}) for soils by high performance liquid chromatography. *Chemosphere.* 17(1):67-77.

Huggenberger, F.J. Letey, W.J. Farmer. 1972. Observed and calculated distribution of lindane in soil columns as influenced by water movement. *Soil Sci. Soc. Am. Proc.* 36:544-548.

Hutzler, N.J., J.C. Crittenden, J.L. Oravitz and P.A. Schaepe. 1983. Groundwater transport of chlorinated organic compounds. *In: American Chemical Society, Div. Environ. Chem., 186th National Meeting.* 23:499-502.

Hutzler, N.J., J.C. Crittenden, and J. S. Gierke. 1986. Transport of organic compounds with saturated groundwater flow: experimental results. *Water Resources Res*. 22(3):285-295.

Johnson-Logan, L.R., R.E. Broshears, and S.J. Klaine. 1992. Partitioning behavior and the mobility of chlordane in groundwater. *Environ. Sci. Technol.* 26(11):2234-2239.

Jury, W.A., W.J. Farmer, and W.F. Spencer. 1984. Behavior assessment model for trace organics in soil: II. Chemical classification and parameter sensitivity. *J. Environ. Qual.* 13(4):567-572.

Jury, W.A., D Russo, G.Streile, and H.E. Abd. 1990. Evaluation of volatilization by organic chemicals residing below the soil surface. *Water Resources Res.* 26(1):13-20.

Kan, A.T., and M.B.Tomson. 1990. Ground water transport of hydrophobic organic compounds in the presence of dissolved organic matter. *Environ. Toxicol. Chem.* 9:253-263.

Karickhoff, S.W. 1981. Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. *Chemosphere*. 10(8):833-846.

Karickhoff, S.W. 1982. Sorption kinetics of hydrophobic pollutants in natural sediments. *Contaminants and Sediments*. 2:193-205.

Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. Sorption of hydrophobic pollutants on natural sediments. *Water Res.* 13:241-248.

Karickhoff, S.W., and K.R.Morris. 1985a. Impact of tubificid oligochaetes on pollutant transport in bottom sediments. *Environ. Sci. Tech.* 19:51-56.

Karickhoff, S.W., and K.R. Morris. 1985b. Sorption dynamics of hydrophobic pollutants in sediment suspensions. *Environ. Toxicol. Chem.* 4:469-479.

Kay, B.D., and D.E. Elrick. 1967. Adsorption and movement of lindane in soils. *Soil Science.* 104:314.

Kishi, H., N. Kogure, and Y. Hashimoto. 1990. Contribution of soil constituents in adsorption coefficient of aromatic compounds, halogenated alicyclic and aromatic compounds to soil. *Chemosphere.* 21(7):867-876.

Koch, R. 1983. Molecular connectivity index for assessing ecotoxicological behaviour of organic compounds. *Toxicol. Environ. Chem.* 6:87-96.

Landrum, P.F., S.R. Nihart, B.J. Eadie, and W.S. Gardner. 1984. Reverse-phase separation method for determining pollutant binding to aldrich humic acid and dissolved organic carbon of natural waters. *Environ. Sci. Technol.* 18(3):187-192.

Lee, J.F., J.R. Crum, and S.A. Boyd. 1989. Enhances retention of organic contaminants by soils exchanged with organic cations. *Environ. Sci. Technol.* 23(11):1365-1372.

Leistra, M. 1970. Distribution of 1,3-dichloropropene over the phases in soil. *J.Agr. Food Chem.* 18(6):1124-1126.

Loch, J.P.G., H.J. Kool, P. Lagas, and J.H.A.M. Verheul. 1986. Removal and retention of volatile chlorinated hydrocarbons in the soils' unsaturated zone. *In: Contaminated Soil.* J.W. Assink and W.J. van der Brink, eds. Matinus Nijhoff Publishers, Dordrecht, Netherlands. 63-77.

Lokke, H. 1984. Sorption of selected organic pollutants in Danish soils. *Ecotoxicol. Environ. Safety* 8:395-409.

Lord, K.A., G.G. Briggs, M.C. Neale, and R. Manlove. 1980. Uptake of pesticides from water and soil by earthworms. *Pest. Sci. 11:401-408.*

Lotse, E.J., D.A. Graetz, G. Chesters, G.B. Lee, and L.W. Newland. 1968. *Environ. Sci. Technol.* 2:353.

Mackay, D., W. Y. Shiu, and K. C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCB's*. Lewis Publishers, Boca Raton, FL.

Mackay, D., W. Y. Shiu, and K. C. Ma. 1993. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume III - Volatile Organic Chemicals.* Lewis Publishers, Boca Raton, FL.

McCall, P.J., R.L. Swann, D.A. Laskowski, S.M. Unger, S.A. Vrona, and H.J. Dishburger. 1980. Estimation of chemical mobility in soil from liquid chromatographic retention times. *Bull. Environ. Contam. Toxicol.* 24:190-195.

McCall, P.J., R.L. Swann, D.A. Laskowski. 1983. Partition models for equilibrium distribution of chemicals in environmental compartments. *In: Fate of Chemicals in the Environment.* R. L. Swann and A. Eschenroeder, eds. ACS Symposium Series 225. American Chemical Society, Washington, DC. 105-123.

McCarthy, J.F., and B.D.Jimenez. 1985. Interactions between polycyclic aromatic hydrocarbons and dissolved humic material: binding and dissociation. *Environ. Sci. Technol.* 19(11):1072-1076.

Means, J.C., S.G. Wood, J.J. Hassett, and W.L. Banwart, 1980. Sorption of polynuclear aromatic hydrocarbons by sediments and soils. *Environ. Sci. Technol.* 14(12):1524-1528.

Meylan, W., P.H. Howard, and R.S. Boethling. 1992. Molecular topology/fragment contribution method for predicting soil sorption coefficients. *Environ. Sci. Technol.,* 26(8):1560-1567.

Miller, C.T., and W.J. Weber, Jr. 1986. Sorption of hydrophobic organic pollutants in saturated soil systems. *J. Cont. Hydrol.* 1(1/2):243-261.

Mills, A.C., and J.W. Biggar. 1969a. Adsorption of gamma-BHC from solutions on several selected adsorbents. *J. Agric. Food Chem.* 17(3):604-608.

Mills, A.C., and J.W. Biggar. 1969b. Solubility-temperature effects on the adsorption of gamma- and beta-BHC from aqueous and hexane solutions by soil materials. *Soil Sci. Soc. Amer. Proc.* 33:210-216.

Moreale, A., and R. van Bladel. 1978. Adsorption et migration du lindane (1,2,3,4,5,6-hexachlorohexane) dans les sols. *Parasitica*. 34(4):233-255.

Paviostathis, S.G. , and K. Jaglal. 1991. Desorptive behavior of trichloroethylene in contaminated soil. *Environ. Sci. Technol.* 25(2):274-279.

Paviostathis, S.G., and G.N. Mathavan. 1992. Desorption kinetics of selected volatile organic compounds from field contaminated soils. *Environ. Sci. Technol.* 26(3):532-538.

Pignatello, J.J. 1990. Slowly reversible sorption of aliphatic halocarbons in soils. I. formation of residual fractions. *Environ. Toxicol. Chem.* 9:1107-1115.

Pignatello, J.J. 1991. Desorption of tetrachloroethene and 1,2-dibromo-3-chloropropane from aquifer sediments. *Environ. Toxicol. Chem. 10:1399-1404.*

Piwoni, M.D., and P. Banerjee. 1989. Sorption of volatile organic solvents from aqueous solution onto subsurface solids. *J. Contam. Hydrol.* 4(2):163-179.

Podoll, R.T., K.C. Irwin, and H.J. Parish. 1989. Dynamic studies of naphthalene sorption on soil from aqueous solution. *Chemosphere*. 18(11/12):2399-2412.

Reinbold, K.A., J.J. Hassett, J.C. Means, and W.L. Banwart. 1979. *Adsorption of Energy-Related Organic Pollutants: A Literature Review*. EPA 600/3-79-086. U.S. Environmental Protection Agency. Washington, DC.

Rippen, G., M. Ilgenstein, W. Klopffer, and H.J. Poremski. 1982. Screening of the adsorption behavior of new chemicals: natural soils and model adsorbents. *Ecotoxicol. Environ. Safety* 6:236-245.

Roberts, P.V., P.L. McCarty, M. Reinhard, and J. Schreiner. 1980. Organic contaminant behavior during groundwater recharge. *Water Poll. Control Fed. J.* 52:161-172.

Rogers, R.D., J.C. McFarlane, and A.J. Cross. 1980. Adsorption and desorption of benzene in two soils and montmorillonite clay. *J. Am. Chem. Soc.* 14(4):457-460.

Rogers, R.D., and J.C. McFarlane. 1981. Sorption of carbon tetrachloride, ethylene dibromide, and trichloroethylene on soil and clay. *Environ. Monitoring and Assessment.* 1:155-162.

Roy, W.R., I. G. Krapac, S. F. J. Chou, and R. A. Griffin. 1987. *Batch-Type Adsorption Procedures for Estimating Soil Attenuation of Chemicals.* Draft Technical Resource Document. EPA/530-SW-87-006. U. S. Environmental Protection Agency. Office of Research and Development. Cincinnati, OH. NTIS PB87-146155.

Russell, D.J., and B. McDuffie. 1986. Chemodynamic properties of phthalate esters: partitioning and soil migration. *Chemosphere.* 15(8):1003-1021.

Rutherford, D.W., and C.T. Chiou. 1992. Effect of water saturation in soil organic matter on the partition of organic compounds. *Environ. Sci. Technol.* 26:965-970.

Rutherford, D.W., C.T. Chiou, and D.E. Kile. 1992. Influence of soil organic matter composition on the partition of organic compounds. *Environ. Sci. Technol.* 26:336-340.

Scheunert, I., E. Topp, A. Attar, and F. Korte. 1994. Uptake pathways of chlorobenzenes in plants and their correlation with *n*-octanol/water partition coefficients. *Ecotoxicol. Environ. Safety*. 27:90-104.

Schwarzenbach, R.P., and J. Westall. 1981. Transport of nonpolar organic compounds from surface water to groundwater. Laboratory sorption studies. *Environ. Sci. Technol.* 15(11):1360-1367.

Schwille, F. 1988. *Dense Chlorinated Solvents in Porous and Fractured Media.* Lewis Publishers, Chelsea, MI.

Seip, H.M., J. Alstad, G.E. Carlberg, K. Martinsen, and R. Skanne. 1986. Measurement of mobility of organic compounds in soils. *Sci. Total Environ.* 50:87-101.

Sharom, M.S., J.R.W. Miles, C.R. Harris, and F.L. McEwen. 1980. Behaviour of 12 insecticides in soil and aqueous suspensions of soil and sediment. *Water Res.* 14:1095-1100.

Smith, J.A., C.T. Chiou, J.A. Kammer, and D.E. Kile. 1990. Effect of soil moisture on sorption of trichloroethene vapor to vadose-zone soil at Picatinny Arsenal, New Jersey. *Environ. Sci. Technol.* 24(5):676-698.

Smith, J.H., W.R. Mabey, N. Bohonos, B.R. Holt, S.S. Lee, T.-W. Chou, D.C. Bomberger, and T. Mill. 1978. *Environmental Pathways of Selected Chemicals in Freshwater Systems. Part 2: Laboratory Studies*. EPA-600/7-78-074. U.S. Environmental Protection Agency, Athens, GA.

Southworth, G.R., and J.L. Keller. 1986. Hydrophobic sorption of polar organics by low organic carbon soils. *Water, Air, and Soil Pollution*. 28:239-248.

Spencer, W.F., and M.M. Cliath. 1970. Desorption of lindane from soil as related to vapor density. *Soil Sci. Soc. Am. Proc.* 34:574-578.

Stauffer, T.B., and W.G. MacIntyre. 1986. Sorption of low-polarity organic compounds on oxide minerals and aquifer material. *Environ. Toxicol. Chem.* 5:949-955.

Szabo, G., S.L. Prosser, and R.A. Bulman. 1990a. Determination of the adsorption coefficient (K_{oc}) of some aromatics for soil by RP-HPLC on two immobilized humic acid phases. *Chemosphere.* 21(6):777-788.

Szabo, G., S.L. Prosser, and R.A. Bulman. 1990b. Prediction of the adsorption coefficient (K_{oc}) for soil by a chemically immobilized humic acid column using RP-HPLC. *Chemosphere.* 21(6):729-739.

Vowles, P.D., and R.F.C. Mantoura. 1987. Sediment-water partition coefficients and HPLC retention factors of aromatic hydrocarbons. *Chemosphere.* 16(1):109-116.

Wahid, P.A., and N. Sethunathan. 1978. A simple method to study pesticide sorption in soils at short time intervals. *Soil Sci.* 126(1):56-58.

Wahid, P.A., and N. Sethunathan. 1979. Sorption-desorption of α, β and γ isomers of hexachlorocyclohexane in soils.*J. Agric. Food Chem.* 27(5):1050-1053

Wahid, P.A., and N. Sethunathan. 1980. Sorption-desorption of lindane by anaerobic and aerobic soils. *J. Agric. Food Chem.* 28(3):623-625.

Wauchope, R.D., T.M. Buttler, A.G. Hornsby, P.W.M. Augustijn-Beckers, and J.P. Burt. 1992. The SRS/ARS/CES pesticide properties database for environmental decision-making. *Rev. Environ. Contam. & Toxicol.* 123:1-164.

Wilson, J.T., C.G. Enfield, W.J. Dunlap, R.L. Cosby, D.A. Foster, and L.B. Baskin. 1981. Transport and fate of selected organic pollutants in a sandy soil. *J. Environ. Qual.* 10(4):501-506.

Wood, A.L., D.C.Bouchard, M.L. Brusseau, and P.S.C. Rao. 1990. Cosolvent effects on sorption and mobility of organic contaminants in soils. *Chemosphere.* 21(4-5):575-587.

Woodburn, K.B., L.S. Lee, P. Suresh, C. Rao, and J.J. Delfino. 1989. Comparison of sorption energetics for hydrophobic organic chemicals by synthetic and natural sorbents from methanol/water solvent mixtures. *Environ. Sci. Technol.* 23:407-413.

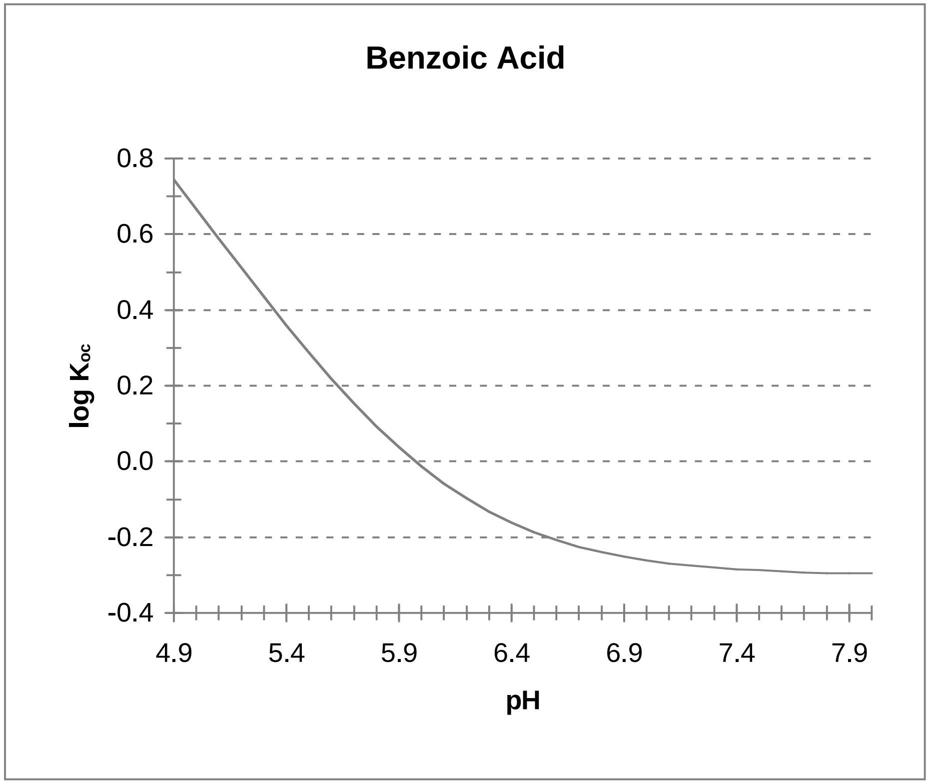
Wu, S., and P.M. Gschwend. 1986. Sorption kinetics of hydrophobic organic compounds to natural sediments and soils. *Environ. Sci. Technol.* 20:717-725.

APPENDIX L

K_{oc} Values for Ionizing Organics as a Function of pH

Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

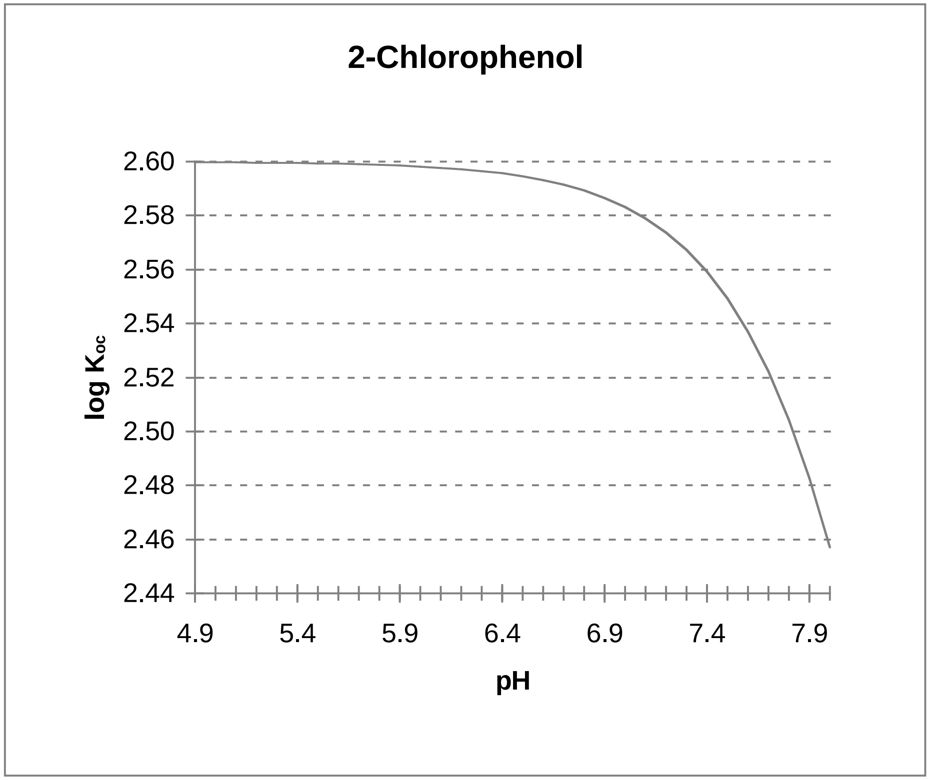
$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
32	4.9	4.18	0.1600	0.5	5.5	0.74
32	5.0	4.18	0.1315	0.5	4.6	0.67
32	5.1	4.18	0.1073	0.5	3.9	0.59
32	5.2	4.18	0.0872	0.5	3.2	0.51
32	5.3	4.18	0.0705	0.5	2.7	0.43
32	5.4	4.18	0.0568	0.5	2.3	0.36
32	5.5	4.18	0.0457	0.5	1.9	0.29
32	5.6	4.18	0.0366	0.5	1.7	0.22
32	5.7	4.18	0.0293	0.5	1.4	0.15
32	5.8	4.18	0.0234	0.5	1.2	0.09
32	5.9	4.18	0.0187	0.5	1.1	0.04
32	6.0	4.18	0.0149	0.5	1.0	-0.01
32	6.1	4.18	0.0119	0.5	0.9	-0.06
32	6.2	4.18	0.0095	0.5	0.8	-0.10
32	6.3	4.18	0.0075	0.5	0.7	-0.13
32	6.4	4.18	0.0060	0.5	0.7	-0.16
32	6.5	4.18	0.0048	0.5	0.7	-0.19
32	6.6	4.18	0.0038	0.5	0.6	-0.21
32	6.7	4.18	0.0030	0.5	0.6	-0.23
32	6.8	4.18	0.0024	0.5	0.6	-0.24
32	6.9	4.18	0.0019	0.5	0.6	-0.25
32	7.0	4.18	0.0015	0.5	0.5	-0.26
32	7.1	4.18	0.0012	0.5	0.5	-0.27
32	7.2	4.18	0.0010	0.5	0.5	-0.27
32	7.3	4.18	0.0008	0.5	0.5	-0.28
32	7.4	4.18	0.0006	0.5	0.5	-0.28
32	7.5	4.18	0.0005	0.5	0.5	-0.29
32	7.6	4.18	0.0004	0.5	0.5	-0.29
32	7.7	4.18	0.0003	0.5	0.5	-0.29
32	7.8	4.18	0.0002	0.5	0.5	-0.30
32	7.9	4.18	0.0002	0.5	0.5	-0.30
32	8.0	4.18	0.0002	0.5	0.5	-0.30



Benzoic Acid

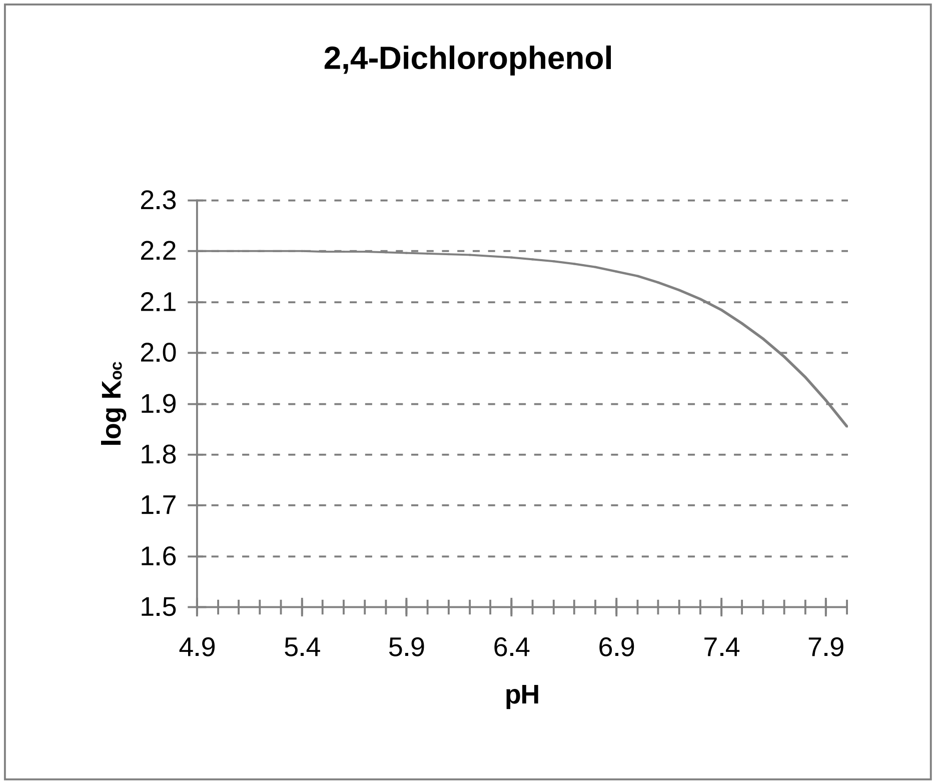
Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
398	4.9	8.40	0.9997	6	398	2.60
398	5.0	8.40	0.9996	6	398	2.60
398	5.1	8.40	0.9995	6	398	2.60
398	5.2	8.40	0.9994	6	398	2.60
398	5.3	8.40	0.9992	6	398	2.60
398	5.4	8.40	0.9990	6	398	2.60
398	5.5	8.40	0.9987	6	397	2.60
398	5.6	8.40	0.9984	6	397	2.60
398	5.7	8.40	0.9980	6	397	2.60
398	5.8	8.40	0.9975	6	397	2.60
398	5.9	8.40	0.9968	6	397	2.60
398	6.0	8.40	0.9960	6	396	2.60
398	6.1	8.40	0.9950	6	396	2.60
398	6.2	8.40	0.9937	6	396	2.60
398	6.3	8.40	0.9921	6	395	2.60
398	6.4	8.40	0.9901	6	394	2.60
398	6.5	8.40	0.9876	6	393	2.59
398	6.6	8.40	0.9844	6	392	2.59
398	6.7	8.40	0.9804	6	390	2.59
398	6.8	8.40	0.9755	6	388	2.59
398	6.9	8.40	0.9693	6	386	2.59
398	7.0	8.40	0.9617	6	383	2.58
398	7.1	8.40	0.9523	6	379	2.58
398	7.2	8.40	0.9406	6	375	2.57
398	7.3	8.40	0.9264	6	369	2.57
398	7.4	8.40	0.9091	6	362	2.56
398	7.5	8.40	0.8882	6	354	2.55
398	7.6	8.40	0.8632	6	344	2.54
398	7.7	8.40	0.8337	6	333	2.52
398	7.8	8.40	0.7992	6	319	2.50
398	7.9	8.40	0.7597	6	304	2.48
398	8.0	8.40	0.7153	6	286	2.46



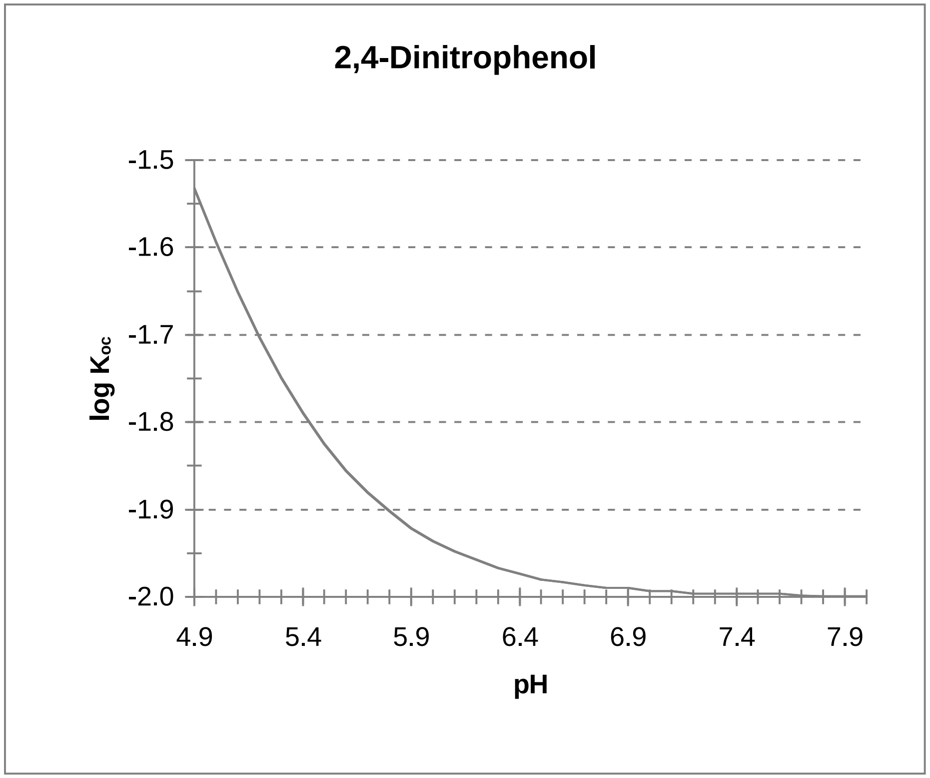
Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
159	4.9	7.90	0.9990	2.4	159	2.20
159	5.0	7.90	0.9987	2.4	159	2.20
159	5.1	7.90	0.9984	2.4	159	2.20
159	5.2	7.90	0.9980	2.4	159	2.20
159	5.3	7.90	0.9975	2.4	159	2.20
159	5.4	7.90	0.9968	2.4	158	2.20
159	5.5	7.90	0.9960	2.4	158	2.20
159	5.6	7.90	0.9950	2.4	158	2.20
159	5.7	7.90	0.9937	2.4	158	2.20
159	5.8	7.90	0.9921	2.4	158	2.20
159	5.9	7.90	0.9901	2.4	157	2.20
159	6.0	7.90	0.9876	2.4	157	2.20
159	6.1	7.90	0.9844	2.4	157	2.19
159	6.2	7.90	0.9804	2.4	156	2.19
159	6.3	7.90	0.9755	2.4	155	2.19
159	6.4	7.90	0.9693	2.4	154	2.19
159	6.5	7.90	0.9617	2.4	153	2.18
159	6.6	7.90	0.9523	2.4	152	2.18
159	6.7	7.90	0.9406	2.4	150	2.18
159	6.8	7.90	0.9264	2.4	147	2.17
159	6.9	7.90	0.9091	2.4	145	2.16
159	7.0	7.90	0.8882	2.4	141	2.15
159	7.1	7.90	0.8632	2.4	138	2.14
159	7.2	7.90	0.8337	2.4	133	2.12
159	7.3	7.90	0.7992	2.4	128	2.11
159	7.4	7.90	0.7597	2.4	121	2.08
159	7.5	7.90	0.7153	2.4	114	2.06
159	7.6	7.90	0.6661	2.4	107	2.03
159	7.7	7.90	0.6131	2.4	98	1.99
159	7.8	7.90	0.5573	2.4	90	1.95
159	7.9	7.90	0.5000	2.4	81	1.91
159	8.0	7.90	0.4427	2.4	72	1.86



Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

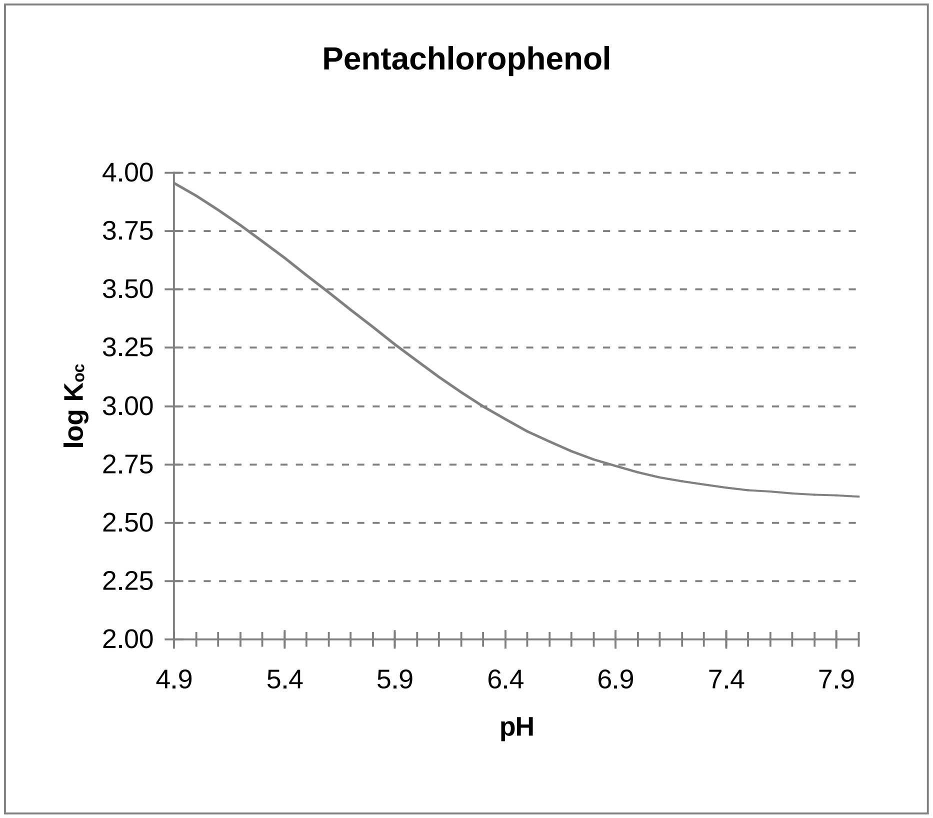
$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
0.8	4.9	3.30	0.0245	0.01	0.03	-1.53
0.8	5.0	3.30	0.0196	0.01	0.03	-1.59
0.8	5.1	3.30	0.0156	0.01	0.02	-1.65
0.8	5.2	3.30	0.0124	0.01	0.02	-1.70
0.8	5.3	3.30	0.0099	0.01	0.02	-1.75
0.8	5.4	3.30	0.0079	0.01	0.02	-1.79
0.8	5.5	3.30	0.0063	0.01	0.01	-1.82
0.8	5.6	3.30	0.0050	0.01	0.01	-1.86
0.8	5.7	3.30	0.0040	0.01	0.01	-1.88
0.8	5.8	3.30	0.0032	0.01	0.01	-1.90
0.8	5.9	3.30	0.0025	0.01	0.01	-1.92
0.8	6.0	3.30	0.0020	0.01	0.01	-1.94
0.8	6.1	3.30	0.0016	0.01	0.01	-1.95
0.8	6.2	3.30	0.0013	0.01	0.01	-1.96
0.8	6.3	3.30	0.0010	0.01	0.01	-1.97
0.8	6.4	3.30	0.0008	0.01	0.01	-1.97
0.8	6.5	3.30	0.0006	0.01	0.01	-1.98
0.8	6.6	3.30	0.0005	0.01	0.01	-1.98
0.8	6.7	3.30	0.0004	0.01	0.01	-1.99
0.8	6.8	3.30	0.0003	0.01	0.01	-1.99
0.8	6.9	3.30	0.0003	0.01	0.01	-1.99
0.8	7.0	3.30	0.0002	0.01	0.01	-1.99
0.8	7.1	3.30	0.0002	0.01	0.01	-1.99
0.8	7.2	3.30	0.0001	0.01	0.01	-2.00
0.8	7.3	3.30	0.0001	0.01	0.01	-2.00
0.8	7.4	3.30	0.0001	0.01	0.01	-2.00
0.8	7.5	3.30	0.0001	0.01	0.01	-2.00
0.8	7.6	3.30	0.0001	0.01	0.01	-2.00
0.8	7.7	3.30	0.00004	0.01	0.01	-2.00
0.8	7.8	3.30	0.00003	0.01	0.01	-2.00
0.8	7.9	3.30	0.00003	0.01	0.01	-2.00
0.8	8.0	3.30	0.00002	0.01	0.01	-2.00



2,4-Dinitrophenol

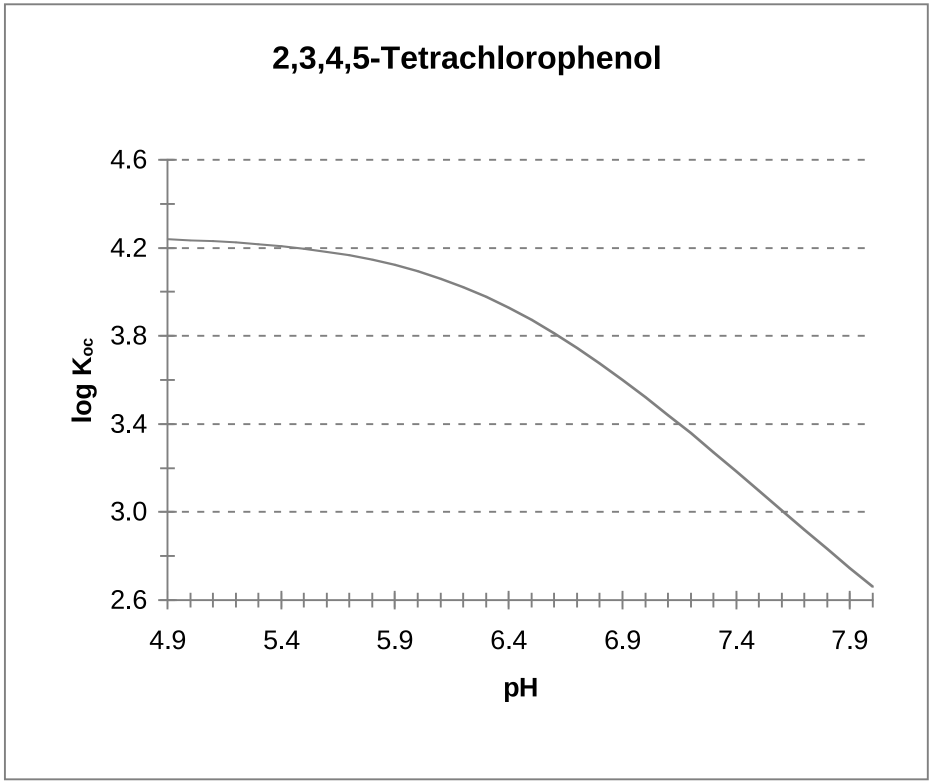
Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
19953	4.9	4.80	0.4427	398	9055	3.96
19953	5.0	4.80	0.3869	398	7964	3.90
19953	5.1	4.80	0.3339	398	6927	3.84
19953	5.2	4.80	0.2847	398	5965	3.78
19953	5.3	4.80	0.2403	398	5097	3.71
19953	5.4	4.80	0.2008	398	4325	3.64
19953	5.5	4.80	0.1663	398	3650	3.56
19953	5.6	4.80	0.1368	398	3073	3.49
19953	5.7	4.80	0.1118	398	2584	3.41
19953	5.8	4.80	0.0909	398	2176	3.34
19953	5.9	4.80	0.0736	398	1837	3.26
19953	6.0	4.80	0.0594	398	1560	3.19
19953	6.1	4.80	0.0477	398	1331	3.12
19953	6.2	4.80	0.0383	398	1147	3.06
19953	6.3	4.80	0.0307	398	998	3.00
19953	6.4	4.80	0.0245	398	877	2.94
19953	6.5	4.80	0.0196	398	781	2.89
19953	6.6	4.80	0.0156	398	703	2.85
19953	6.7	4.80	0.0124	398	640	2.81
19953	6.8	4.80	0.0099	398	592	2.77
19953	6.9	4.80	0.0079	398	552	2.74
19953	7.0	4.80	0.0063	398	521	2.72
19953	7.1	4.80	0.0050	398	496	2.70
19953	7.2	4.80	0.0040	398	476	2.68
19953	7.3	4.80	0.0032	398	461	2.66
19953	7.4	4.80	0.0025	398	447	2.65
19953	7.5	4.80	0.0020	398	437	2.64
19953	7.6	4.80	0.0016	398	429	2.63
19953	7.7	4.80	0.0013	398	423	2.63
19953	7.8	4.80	0.0010	398	418	2.62
19953	7.9	4.80	0.0008	398	414	2.62
19953	8.0	4.80	0.0006	398	410	2.61



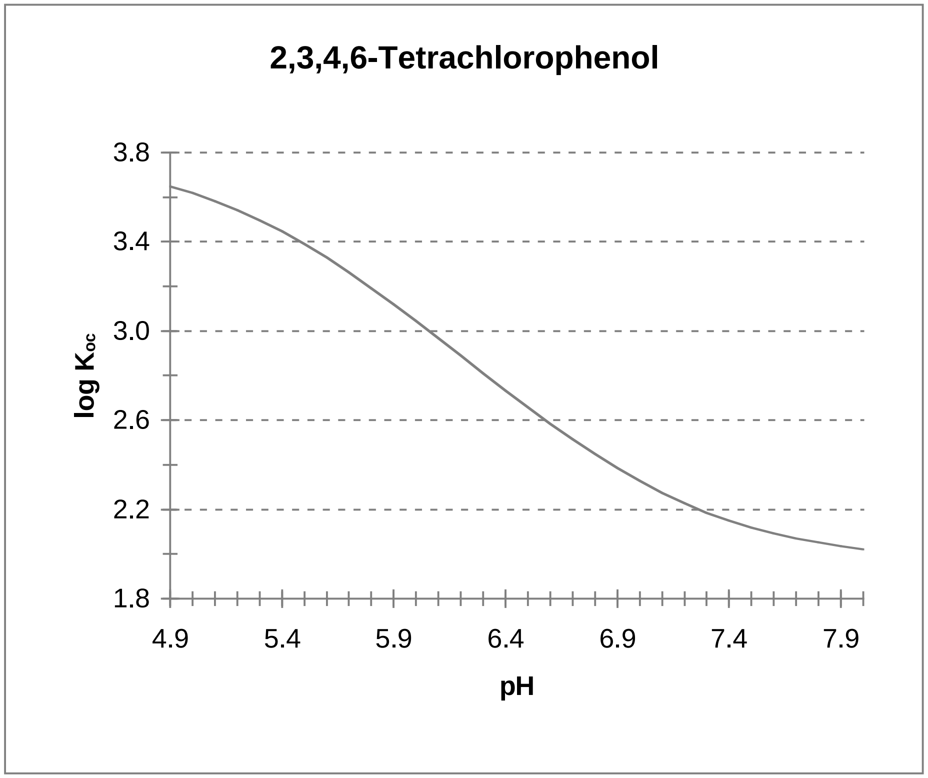
Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
17916	4.9	6.35	0.9657	67	17304	4.24
17916	5.0	6.35	0.9572	67	17152	4.23
17916	5.1	6.35	0.9468	67	16966	4.23
17916	5.2	6.35	0.9339	67	16736	4.22
17916	5.3	6.35	0.9182	67	16456	4.22
17916	5.4	6.35	0.8991	67	16115	4.21
17916	5.5	6.35	0.8762	67	15706	4.20
17916	5.6	6.35	0.8490	67	15221	4.18
17916	5.7	6.35	0.8171	67	14651	4.17
17916	5.8	6.35	0.7801	67	13991	4.15
17916	5.9	6.35	0.7381	67	13241	4.12
17916	6.0	6.35	0.6912	67	12404	4.09
17916	6.1	6.35	0.6401	67	11492	4.06
17916	6.2	6.35	0.5855	67	10518	4.02
17916	6.3	6.35	0.5288	67	9506	3.98
17916	6.4	6.35	0.4712	67	8477	3.93
17916	6.5	6.35	0.4145	67	7465	3.87
17916	6.6	6.35	0.3599	67	6491	3.81
17916	6.7	6.35	0.3088	67	5579	3.75
17916	6.8	6.35	0.2619	67	4742	3.68
17916	6.9	6.35	0.2199	67	3992	3.60
17916	7.0	6.35	0.1829	67	3332	3.52
17916	7.1	6.35	0.1510	67	2762	3.44
17916	7.2	6.35	0.1238	67	2277	3.36
17916	7.3	6.35	0.1009	67	1868	3.27
17916	7.4	6.35	0.0818	67	1527	3.18
17916	7.5	6.35	0.0661	67	1247	3.10
17916	7.6	6.35	0.0532	67	1017	3.01
17916	7.7	6.35	0.0428	67	831	2.92
17916	7.8	6.35	0.0343	67	679	2.83
17916	7.9	6.35	0.0274	67	556	2.75
17916	8.0	6.35	0.0219	67	458	2.66



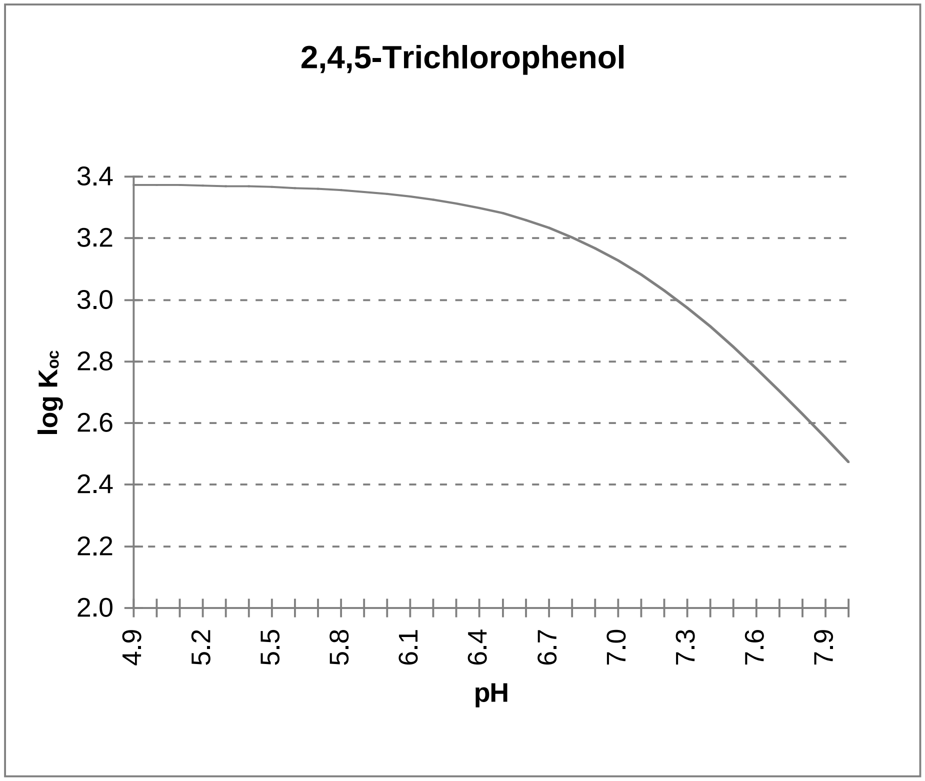
Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
6190	4.9	5.30	0.7153	93	4454	3.65
6190	5.0	5.30	0.6661	93	4154	3.62
6190	5.1	5.30	0.6131	93	3831	3.58
6190	5.2	5.30	0.5573	93	3491	3.54
6190	5.3	5.30	0.5000	93	3142	3.50
6190	5.4	5.30	0.4427	93	2792	3.45
6190	5.5	5.30	0.3869	93	2452	3.39
6190	5.6	5.30	0.3339	93	2129	3.33
6190	5.7	5.30	0.2847	93	1829	3.26
6190	5.8	5.30	0.2403	93	1558	3.19
6190	5.9	5.30	0.2008	93	1317	3.12
6190	6.0	5.30	0.1663	93	1107	3.04
6190	6.1	5.30	0.1368	93	927	2.97
6190	6.2	5.30	0.1118	93	775	2.89
6190	6.3	5.30	0.0909	93	647	2.81
6190	6.4	5.30	0.0736	93	542	2.73
6190	6.5	5.30	0.0594	93	455	2.66
6190	6.6	5.30	0.0477	93	384	2.58
6190	6.7	5.30	0.0383	93	327	2.51
6190	6.8	5.30	0.0307	93	280	2.45
6190	6.9	5.30	0.0245	93	242	2.38
6190	7.0	5.30	0.0196	93	213	2.33
6190	7.1	5.30	0.0156	93	188	2.27
6190	7.2	5.30	0.0124	93	169	2.23
6190	7.3	5.30	0.0099	93	153	2.19
6190	7.4	5.30	0.0079	93	141	2.15
6190	7.5	5.30	0.0063	93	131	2.12
6190	7.6	5.30	0.0050	93	123	2.09
6190	7.7	5.30	0.0040	93	117	2.07
6190	7.8	5.30	0.0032	93	113	2.05
6190	7.9	5.30	0.0025	93	108	2.03
6190	8.0	5.30	0.0020	93	105	2.02


2,3,4,6-Tetrachlorophenol

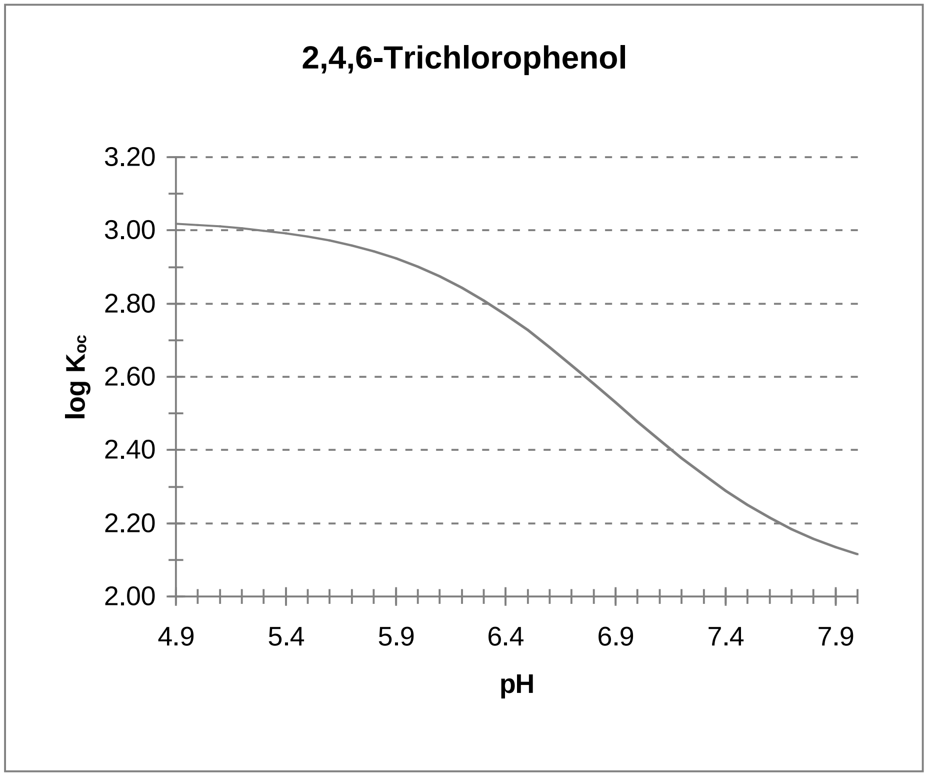
Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
2380	4.9	7.10	0.9937	36	2365	3.37
2380	5.0	7.10	0.9921	36	2361	3.37
2380	5.1	7.10	0.9901	36	2357	3.37
2380	5.2	7.10	0.9876	36	2351	3.37
2380	5.3	7.10	0.9844	36	2343	3.37
2380	5.4	7.10	0.9804	36	2334	3.37
2380	5.5	7.10	0.9755	36	2323	3.37
2380	5.6	7.10	0.9693	36	2308	3.36
2380	5.7	7.10	0.9617	36	2290	3.36
2380	5.8	7.10	0.9523	36	2268	3.36
2380	5.9	7.10	0.9406	36	2241	3.35
2380	6.0	7.10	0.9264	36	2207	3.34
2380	6.1	7.10	0.9091	36	2167	3.34
2380	6.2	7.10	0.8882	36	2118	3.33
2380	6.3	7.10	0.8632	36	2059	3.31
2380	6.4	7.10	0.8337	36	1990	3.30
2380	6.5	7.10	0.7992	36	1909	3.28
2380	6.6	7.10	0.7597	36	1817	3.26
2380	6.7	7.10	0.7153	36	1713	3.23
2380	6.8	7.10	0.6661	36	1597	3.20
2380	6.9	7.10	0.6131	36	1473	3.17
2380	7.0	7.10	0.5573	36	1342	3.13
2380	7.1	7.10	0.5000	36	1208	3.08
2380	7.2	7.10	0.4427	36	1074	3.03
2380	7.3	7.10	0.3869	36	943	2.97
2380	7.4	7.10	0.3339	36	819	2.91
2380	7.5	7.10	0.2847	36	703	2.85
2380	7.6	7.10	0.2403	36	599	2.78
2380	7.7	7.10	0.2008	36	507	2.70
2380	7.8	7.10	0.1663	36	426	2.63
2380	7.9	7.10	0.1368	36	357	2.55
2380	8.0	7.10	0.1118	36	298	2.47


2,4,5-Trichlorophenol

Appendix L. K_{oc} Values for Ionizing Organics as a Function of pH

$K_{oc,n}$	pH	pKa	Φ	$K_{oc,i}$	K_{oc}	log K_{oc}
1070	4.9	6.40	0.9693	107	1040	3.02
1070	5.0	6.40	0.9617	107	1033	3.01
1070	5.1	6.40	0.9523	107	1024	3.01
1070	5.2	6.40	0.9406	107	1013	3.01
1070	5.3	6.40	0.9264	107	999	3.00
1070	5.4	6.40	0.9091	107	982	2.99
1070	5.5	6.40	0.8882	107	962	2.98
1070	5.6	6.40	0.8632	107	938	2.97
1070	5.7	6.40	0.8337	107	910	2.96
1070	5.8	6.40	0.7992	107	877	2.94
1070	5.9	6.40	0.7597	107	839	2.92
1070	6.0	6.40	0.7153	107	796	2.90
1070	6.1	6.40	0.6661	107	748	2.87
1070	6.2	6.40	0.6131	107	697	2.84
1070	6.3	6.40	0.5573	107	644	2.81
1070	6.4	6.40	0.5000	107	589	2.77
1070	6.5	6.40	0.4427	107	533	2.73
1070	6.6	6.40	0.3869	107	480	2.68
1070	6.7	6.40	0.3339	107	429	2.63
1070	6.8	6.40	0.2847	107	381	2.58
1070	6.9	6.40	0.2403	107	338	2.53
1070	7.0	6.40	0.2008	107	300	2.48
1070	7.1	6.40	0.1663	107	267	2.43
1070	7.2	6.40	0.1368	107	239	2.38
1070	7.3	6.40	0.1118	107	215	2.33
1070	7.4	6.40	0.0909	107	195	2.29
1070	7.5	6.40	0.0736	107	178	2.25
1070	7.6	6.40	0.0594	107	164	2.22
1070	7.7	6.40	0.0477	107	153	2.18
1070	7.8	6.40	0.0383	107	144	2.16
1070	7.9	6.40	0.0307	107	137	2.14
1070	8.0	6.40	0.0245	107	131	2.12



APPENDIX M

Response to Peer-Review Comments on MINTEQA2 Model Results

APPENDIX M

Response to Peer-Review Comments on MINTEQA2 Model Results

Peer review of the SSL MINTEQA2 model results identified several issues of concern, including

- The charge balance exceeds an acceptable margin of difference (5 percent) in most of the simulations. A variance in excess of 5 percent may indicate that the model problem is not correctly chemically poised and therefore the results may not be chemically meaningful.
- The model should not allow sulfate to adsorb to the iron oxide. Sulfate is a weakly outer-sphere adsorbing species and by including the adsorption reaction, sulfate is removed from the aqueous phase at pH values less than 7 and is prevented from participating in precipitation reaction at these pH values.
- Modeled K_d values for barium and zinc could not be reproduced for all studied conditions.

The remainder of this Appendix addresses each of these issues.

Charge balance in the MINTEQA2 model runs

Although the charge imbalances (e.g., 6.8% at pH 8.0 and 54.9% at pH 4.9) are present especially at high and low pH conditions, the conclusion that the charge imbalance makes the model results not chemically meaningful is not warranted.

MINTEQA2 uses two primary equations to solve chemical equilibrium problems: the mass action equation (also called the mass law equation) and the mass balance equation. MINTEQA2 does not use the charge balance equation to obtain the mathematical solution of the equilibrium problem. This does not mean that the charge balance equation has no meaning in MINTEQA2 calculations.

The reviewer's concern is understandable. It is logical that any chemical system whose charges are not in balance must be incomplete or have erroneous concentrations for one or more components. However, the systems being modeled here are not "real" systems in the sense that they physically exist somewhere so that measurements can be made on them. Rather, they are generic, representative systems for ground water with variable (high, medium, low) concentrations of those parameters that most significantly impact K_d.

The modeled groundwater consists of national median concentrations of those major cations and anions that are most likely to impact the chemistry of the trace metal of interest by: (1) their complexation with the trace metal, (2) their competition with the trace metal for sorption sites, and/or (3) their effect on the ionic strength of the solution and thus, the activity coefficients of all species in solution including the trace metal. The settings of the three components of this representative system that have the greatest impact on the calculated K_d for various trace metals are systematically varied. The three "master variable" components are pH, iron hydroxide sorption site concentration, and concentration of natural organic matter (particulate and dissolved).

No attempt was made to reconcile charge balances at the different settings of the three master variables. If reconciling charge balance had been attempted, it would have been accomplished by adjusting the concentrations of relatively inert anions and cations (e.g., NO_3^-, Na^+) as needed to balance the charge at equilibrium. It would be unwise to adjust the concentrations of more reactive components (e.g., CO_3^{2-}, Ca^{2+}). To do so would be inconsistent with the initial assumption that those constituents could be adequately represented by median concentrations observed in ground water and that variability in the system could be captured by varying the three master components.

Table M-1 shows the result if the concentrations of the less reactive components NO_3^- and Na^+ are adjusted in the high and low pH model runs so as to give a charge imbalance of <5% at equilibrium. The results shown pertain to the medium iron hydroxide and medium natural organic matter settings for zinc at the pH values listed. As shown in the table, the K_d values computed differ little from those presented in this report. The expected degree of error in the K_d values due to the many simplifications and assumptions involved in generic modeling must surely exceed the variance due to charge imbalance.

Table M-1. K_d values with and without counter ions (Na^+ or NO_3^-) added to balance charge.

pH	K_d[1] (L/kg) No Counter Ion Added	K_d[1] (L/kg) With Na^+ or NO_3^- Added
4.9	1.61	1.51
8.0	16,161	16,135

[1] K_d values shown correspond to the medium iron hydroxide, medium natural organic matter settings. Counter ions were added to reduce charge imbalance to <5% at equilibrium.

Sulfate adsorption in MINTEQA2 model runs

The peer reviewer states that sulfate should not be allowed to adsorb to the iron oxide. The reviewer concludes that by including the adsorption reactions "sulfate is removed from the aqueous phase at pH values less than 7 and is prevented from participating in precipitation reactions at these pH values".

The sulfate adsorption reactions on iron oxide included in the MINTEQA2 model runs were taken from a database of adsorption reactions that has been shown to give reliable results in predicting sulfate adsorption on pure phase iron oxide (Dzombak, 1986). The reviewer is correct in that free sulfate concentration is enhanced at low pH in runs without sulfate adsorption relative to runs with sulfate adsorption. However, for runs with low contaminant trace metal concentrations from which the SSL K_d's were taken, metal-sulfate precipitates do not form regardless of whether sulfate adsorption is included or not. Also, the K_d values over the entire range of trace metal concentrations modeled do not differ significantly when sulfate adsorption is included versus excluded.

Test runs were conducted on barium, zinc and cadmium at various settings of the three master variables (pH, natural organic matter (NOM) concentration, and iron oxide (FeOX) sorption site concentration). Table M-2 shows the K_d values for the lowest and highest trace metal concentration for model runs with and without sulfate adsorption. Results are shown for barium, zinc and cadmium at the indicated settings of the master variables. Where results differ for the "with" and "without" sulfate adsorption cases, it is most frequently due to the formation of aqueous complexes between the trace metal and sulfate that compete with trace metal adsorption reactions, especially at low metal concentrations.

Table M-2. K_d values calculated with and without sulfate adsorption reactions.

Metal (settings)	K_d^1 (L/kg) with SO_4 adsorption	K_d^1 (L/kg) without SO_4 adsorption
Ba (MMH)	2.01 - 0.10	2.01 - 0.10
Ba (MMM)	1.37 - 0.04	1.37 - 0.04
Ba (LMM)	0.59 - 0.04	0.59 - 0.04
Ba (LLM)	0.12 - 0.01	0.12 - 0.01
Ba (LLL)	0.12 - 0.01	0.12 - 0.01
Zn (MMH)	1537 - 863	1478 - 830
Zn (LMM)	1.61 - 0.42	1.57 - 0.41
Zn (LML)	1.46 - 0.26	1.43 - 0.25
Cd (LMM)	0.94 - 0.01	0.91 - 0.01

[1] K_d range shown corresponds to the lowest and highest trace metal concentrations. Master variable settings are indicated by a three letter code for each model run: the leftmost letter indicates pH, the middle letter represents the NOM concentration, and the rightmost letter indicates the concentration of FeOX adsorption sites (eg., HLM indicates high pH, low natural organic matter, medium and iron oxide site concentration).

Reproducing RTI results for barium and zinc

The peer reviewer had difficulty reproducing the K_d values computed for barium and zinc. The reviewer included two sample input files for MINTEQA2 that had failed to produce results similar to the SSL calculations.

The SSL results can be reproduced for all metals using the current version of MINTEQA2 (v3.11) distributed by EPA. As indicated in the 1994 Technical Background Document, a modified version of this model was used to calculate SSL K_ds. The current version can be used to calculate the same results by performing the following steps:

1) Edit the v3.11 component database file COMP.DBS to insert a component to represent particulate organic matter (POM). Use the 3-digit identifying number 251, a charge of -2.8, and a molar mass of zero.
2) Edit the v3.11 file THERMO.DBS to add the metal POM reactions shown in Appendix H of the RTI draft report. The file DATABASE.DOC included with MINTEQA2 v3.11 gives detailed instructions for modifying the database file. After all reactions are added, del or rename the current THERMO.UNF and TYPE6.UNF files and execute program UNFRMT (included with v3.11) to create new *.UNF files.

3) Observe that there were two modifications to v3.11 that make calculation of K_d in L/kg easier in the version used by RTI. Since those modifications are not present in v3.11 itself, the user must take care in computing K_d. The procedure is to first obtain the calculated concentration of the metal of interest (say, barium) bound with POM from PART 3 of the output file. If you have set the solid precipitation flag to print a report each time a solid precipitates or dissolves, there will be a series of PART 3 outputs each corresponding to a precipitation or dissolution event. You must be sure that the PART 3 output from which you obtain the metal-POM concentration is the equilibrium output (i.e., it occurs prior to the PART 5 EQUILIBRATED MASS DISTRIBUTION with no intervening PROVISIONAL MASS DISTRIBUTION). After obtaining the metal-POM concentration, locate the line corresponding to the trace metal of interest, say barium in the PART 5 EQUILIBRATED MASS DISTRIBUTION section. Obtain the total sorbed concentration value and to this value add the concentration of metal-POM species. This is necessary because v3.11 recognizes only components with number 811 through 859 as sorption components. The metal-POM concentration will not have been added in the sorbed column. It will instead have been included in the dissolved column, so subtract the metal-POM concentration from the dissolved total. Finally, to compute K_d, take the ratio of sorbed over dissolved (after the adjustment for metal-POM). The resulting K_d must be divided by 3.1778 kg/L (the mass of soil that one liter of solution is equilibrated with) to express the result in L/kg.

If the above three steps are followed, the v3.11 MINTEQA2 will give the same result as in the 1994 Technical Background Document provided the data in the input file is correct. The two input files sent designed by the reviewer did not give correct results even when these steps were followed because of faulty values in the input file. The files supplied by the reviewer (SSLBA.INP and SSLZN.INP) were correct in all respects except two:

1) The site concentration for the POM component at the medium setting was entered as 1.930×10^3 mg/L. This value was evidently obtained from the table on page 33 of the EPA report (US EPA, 1992) after converting to mg/L. This is not the correct value for this the POM component. The correct value is 9.31×10^{-4} mol/l and is found in the table on page 38 of EPA report.

2) The iron oxide adsorbent is represented by two site types (components 811 and 812). The high population site has a lower affinity for the iron oxide surface for metals (expressed in a smaller log K in the adsorption reactions involving metals). For a particular metal, say, zinc, it will be noted that there are two reactions in the database of 42 iron oxide adsorption reactions (FEW-DLM.DBS). This three-digit component number associated with the reaction having the smaller log K of the two is the number to that must be used for the high population site. That is, component 812 should be entered at the higher site concentration and 811 at the lower site concentration. The set of site concentrations is given on page 44 of the EPA report. In the sample input files, component 811 was associated with the high site concentration and 812 with the lower.

After correcting these two errors and observing the special requirements of using of v3.11 as indicated above, the K_d values obtained using MINTEQA2 v3.11 with the peer reviewer's files were virtually identical to the SSL results.

References

Dzombak, D.A., 1986. Toward a Uniform Model for the Sorption of Inorganic Ions on Hydrous Oxides. Ph.D. Thesis, Massachusetts Institute of Technology, Cambridge, MA.

US EPA (Environmental Protection Agency), 1992. Background Document for Finite Source Methodology for Wastes Containing Metals. HWEP-S0040. Office of Solid Waste, Washington, DC, 68 pages.