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PRESENTED BY Paula Ann Labieniec

Civil and Environmental Engineering and
Engineering and Public Policy

ACCEPTED BY THE DEPARTMENT OF _____

David Zymlak

MAJOR PROFESSOR

8-16-94

DATE

R. A. Lutz

DEPARTMENT HEAD

Sept 3, 94

DATE

V. Granger-Taylor

DEPARTMENT HEAD

94 Sep 8

DATE

APPROVED BY THE COLLEGE COUNCIL

Ch. H. H. H.

DEAN

9-9-94

DATE

MASTER

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CARNEGIE MELLON UNIVERSITY

**THE RISK IMPLICATIONS OF APPROACHES TO
SETTING SOIL REMEDIATION GOALS AT
HAZARDOUS WASTE CONTAMINATED SITES**

A DISSERTATION
SUBMITTED TO THE GRADUATE SCHOOL
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
for the degree of
DOCTOR OF PHILOSOPHY
in
CIVIL AND ENVIRONMENTAL ENGINEERING
and
ENGINEERING AND PUBLIC POLICY

by
PAULA ANN LABIENIEC

Pittsburgh, Pennsylvania 15213
August, 1994

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TABLE OF CONTENTS

Preface	i
Acknowledgments	ii
Abstract	iii
Executive Summary	v
 Chapter One: SoilRisk: A Risk Assessment Model for Organic Contaminants in Soil	
Abstract	1
Introduction.....	2
Overview of SoilRisk	3
Unsaturated zone module	5
Overview.....	5
Contaminant distribution and mass transport equations.....	5
Accounting for a clean soil cover	8
Modification for use in SoilRisk	8
Link to exposure module.....	10
Saturated zone module	10
Assumptions.....	10
Link to the unsaturated zone module	11
Solute transport equations	11
Link to the exposure module	12
Air Dilution/Dispersion module	13
Link to the unsaturated zone module	13
Link to the exposure module	13
Dust generation module	14
Exposure module	15
Exposure scenarios and default assumptions.....	15
Contaminant concentration in indoor air	16
Role of non-consumptive use of water	16
Role of soil-gas infiltration.....	17
Absorbed dose equations	18
Risk module	18
Deterministic or stochastic mode	19
Model availability	20
Summary	20
Acknowledgments	21
References	21
Notation	24
 Chapter Two: Quantitative Evaluation of Uncertainty in a Site-Specific Risk Assessment	
Abstract	33
Introduction.....	34
Methodology	35
Generalized site	35
Contaminants.....	36
Exposure scenarios and routes	37
Risk calculation	38

Characterizing uncertainty in site input parameters	38
Sensitivity analysis	39
Uncertainty analysis	40
Results	41
Sensitivity analysis	41
Uncertainty analysis	46
Summary and conclusions	49
Acknowledgments	51
References	51

Chapter Three: Risk Variability Due To Uniform Soil Remediation

Goals	68
Abstract	68
Introduction	69
Methodology	70
Overview	70
Exposure scenarios	71
Risk calculation	72
Contaminants	72
Application using a DRASTIC Map	72
Development of input distributions	72
Parameters describing the contaminated layer	74
Unsaturated zone parameters	74
Saturated zone parameters	76
Climate and site surface parameters	76
Development of risk distributions	77
Application using preliminary distributions	77
Results	77
Using a DRASTIC Map of a county	78
Using preliminary distributions for a state	80
Summary and Conclusions	81
Acknowledgments	83
References	84

Chapter Four: Establishing and Evaluating the Risk Implications of Uniform Soil Remediation Goals

Uniform Soil Remediation Goals	101
Abstract	101
Introduction	102
Risk variability across sites	104
Establishing uniform soil remediation goals	106
Tailoring the uniform approach to reduce risk variability	107
Summary and conclusions	109
References	110

Chapter Five: Summary, Conclusions, and Recommendations for

Future Research	115
Summary	116
Conclusions	119
Recommendations for future research	119
References	122

List of Appendices

- Appendix A: Review of Existing Models for Exposure Assessment of Contaminated Soil
- Appendix B: SoilRisk: Detailed Equations for the Unsaturated Zone Solute Fate/Transport Module
- Appendix C: SoilRisk: Estimation Method for Compound Diffusion Coefficients and K_H
- Appendix D: SoilRisk: Details of the Dust Generation Module
- Appendix E: Definition of soil used in specifying soil remediation goals
- Appendix F: Review of TCE Contaminated Sites
- Appendix G: Effective Half-Lives of Benzene, TCE, Chlordane, and BAP: A Literature Review
- Appendix H: Site-Specific Sensitivity Analysis Plots
- Appendix I: Frequency Histograms of DRASTIC Parameters for Ross County, Ohio
- Appendix J: Overview and Critique of Current Uniform Approaches to Setting Soil Remediation Goals

PREFACE

The organization of this dissertation requires some explanation. Chapters 1-4 consist of a series of four manuscripts[†] followed by Chapter 5 which provides a summary, conclusions and recommendations for future research. Since each chapter was written as a stand-alone manuscript, there are several peculiarities in their collective presentation as a dissertation. Tables and figures are numbered starting from one in each chapter and appear at the end of the chapter. Some tables and figures appear in more than one chapter. Also, citations of other chapters are made by citing the manuscript, not the chapter. Thus, the reference list in each chapter contains references to the others. The titles of the manuscripts referenced and chapter titles are the same, so this should not cause any confusion. Any supporting material that was not suited for publication, but necessary for background and for documentation of methods and results, appears in a series of appendices. This dissertation and its appendices are cited in the chapters where appropriate.

[†] Chapters 1-3 were prepared as a series of research papers to be submitted to the Journal of Environmental Engineering and Chapter 4 as a discussion paper to be submitted to Environmental Science and Technology, all with David A. Dzombak and Robert L. Siegrist as co-authors (August, 1994).

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ABSTRACT

An integrated exposure and carcinogenic risk assessment model for organic contamination in soil, SoilRisk, was developed and used for evaluating the risk implications of both site-specific and uniform-concentration approaches to setting soil remediation goals at hazardous-waste-contaminated sites. SoilRisk was applied to evaluate the uncertainty in the risk estimate due to uncertainty in site conditions at a representative site. It was also used to evaluate the variability in risk across a region of sites that can occur due to differences in site characteristics that affect contaminant transport and fate when a uniform concentration approach is used. In evaluating regional variability, Ross County, Ohio and the State of Ohio were used as examples. All analyses performed considered four contaminants (benzene, trichloroethylene (TCE), chlordane, and benzo[a]pyrene (BAP)) and four exposure scenarios (commercial, recreational and on- and offsite residential). Regardless of whether uncertainty in risk at a single site or variability in risk across sites was evaluated, the exposure scenario specified and the properties of the target contaminant had more influence than variance in site parameters on the resulting variance and magnitude of the risk estimate. In general, variance in risk was found to be greater for the relatively less degradable and more mobile of the chemicals studied (TCE and chlordane) than for benzene which is highly degradable and BAP which is very immobile in the subsurface. It is concluded that for all contaminants, soil remediation goals should be established with consideration of the exposure scenario. For contaminants that are highly degradable such as benzene, or immobile in the subsurface such as BAP, specifying a single contaminant concentration for a given exposure scenario as a uniform goal can result in relatively small

variance in the regional variability of risk. However, for mobile and persistent compounds like TCE and chlordane, a single contaminant concentration in soil for a given exposure scenario can result in large variance in the regional risk variability. For such compounds, a hybrid approach is proposed that involves the use of selected site characteristics to identify the appropriate soil remediation goal from a matrix of acceptable contaminant concentration levels.

EXECUTIVE SUMMARY

Currently in the U.S., it is common for soil remediation goals to be set on a site-by-site basis to meet a target risk by means of site-specific risk assessment. This site-specific approach has proven to require significant human and financial resources to acquire the necessary site data, perform the risk assessment, and provide regulatory oversight. Many believe that setting uniform, concentration-based soil remediation goals would go far in reducing the amount of time and resources required to complete hazardous waste site investigations and cleanup actions and in improving the consistency of these actions. However, when a single contaminant concentration is used as a soil remediation goal at all potential sites in a region, risk will vary across sites due to differences in exposure conditions and physical/chemical characteristics that affect contaminant fate and transport. Thus, a uniform goal for a particular contaminant could result in some sites whose post-remediation risk exceeds the acceptable risk level and others whose residual risk is lower than the acceptable level, suggesting a less or more stringent soil remediation goal would have been adequate at the respective sites. Despite the fact there is significant interest at the state, national, and even international level in developing uniform approaches, quantitative information regarding the risk implications of alternative approaches to establishing soil remediation goals has been lacking. The purpose of this work has been to develop an integrated carcinogenic risk assessment model for organic contaminants in soil and apply it to evaluate and compare the risk implications of site-specific and uniform approaches to setting soil remediation goals.

After consideration of currently available models, a model was developed to enable deterministic and/or stochastic evaluation of the carcinogenic risk due to organic contamination in soil. The model developed accounts for both volatilization and leaching of the contaminant from soil, and estimates the average contaminant concentrations in the air, soil, and ground water over a specified duration of exposure. Thus, risk due to a number of different exposure routes can be calculated. The first chapter entitled *SoilRisk: A risk assessment model for organic contaminants in soil* describes the model in detail. In Appendix A, an overview and critique of currently available models is presented. It establishes the lack of any currently available models suitable for integrated risk assessment of contaminated soil sites. SoilRisk is the most comprehensive model yet developed for risk assessment of contaminated soil.

A key component of SoilRisk is an analytical model for the fate and transport of organics in unsaturated soil developed by Jury et al.(1983, 1990). In the integrated model developed, chemical losses from the unsaturated zone occur due to first-order degradation, volatilization at the soil surface, and leaching to the saturated zone. The unsaturated zone module is linked to air dilution/dispersion, saturated zone transport, and dust generation modules to allow estimation of long-term average air, groundwater, respirable dust, and soil contaminant concentrations at specified points of exposure. Default assumptions for several different exposure scenarios including recreational, commercial/industrial, and on- and offsite residential were developed based on current U.S. Environmental Protection Agency guidance.

SoilRisk permits estimation of the carcinogenic risk resulting from a specified contaminant concentration in soil, or the contaminant concentration in soil to meet a specified level of risk can be determined. These model outputs can be evaluated as single values or as probability distributions, depending on whether site input parameters are specified

deterministically or probabilistically. When the model is run probabilistically for a specified exposure scenario, exposure parameters and carcinogenic potency slope factors are treated deterministically.

In Chapter Two, *Quantitative Evaluation of Uncertainty in A Site Specific Risk Assessment*, the uncertainty in the carcinogenic risk estimated using SoilRisk due to uncertainty in site conditions at a representative contaminated-soil site was quantified in order to evaluate uncertainty in the site-specific approach to setting soil remediation goals. Sensitivity of the risk estimate to site parameters was also explored. SoilRisk was applied to four different suspected or known human carcinogens chosen to represent a wide range of physical/chemical properties (benzene, trichloroethylene (TCE), chlordane, and benzo[a]pyrene (BAP)) and four exposure scenarios (commercial, recreational and on- and offsite residential). It was shown that the sensitivity of the risk estimate to site conditions varies widely depending on the chemical contaminant and on the specified exposure scenario. As a result, the contaminant properties and the assumed exposure scenario have far more influence than uncertainty in site parameters on the resulting uncertainty and magnitude of the total risk estimate. In general, uncertainty in risk was found to be greater for the relatively less degradable and more mobile of the chemicals studied (TCE and chlordane) than for benzene which is highly degradable and BAP which is very immobile in the subsurface. This difference was attributed to the fact that for the more mobile and persistent compounds, the groundwater exposure routes were predicted to predominate and saturated zone parameters were found to effect a large influence on the risk estimate. The risk estimate for the offsite residential exposure scenario was particularly sensitive to the saturated zone parameters when TCE- and chlordane-contaminated soil were considered.

The third chapter, *Risk Variability Due to Uniform Soil Remediation Goals*, presents a methodology to evaluate the variability in risk estimated using SoilRisk across potential

sites in a region when a single contaminant concentration in soil is used as a uniform remediation goal. Variability in risk from site-to-site can occur due to differences in site characteristics that affect transport and fate. The methodology was applied to a relatively small geographic region for which detailed hydrogeologic information is available (Ross County, Ohio) and to a relatively larger region (the state of Ohio) for which a full characterization of site variability is not yet possible due to lack of information. Four different carcinogenic contaminants (benzene, TCE, chlordane, and BAP) and exposure scenarios (commercial, recreational and on- and offsite residential) were evaluated using SoilRisk. Results are presented in the form of cumulative distribution functions of risk which summarize the variability in risk across the regions analyzed due to variability in site hydrogeologic conditions. Results were found to vary according to the contaminant and exposure scenario considered. In general, for contaminants that are highly degradable such as benzene or immobile in the subsurface such as BAP, specifying a single contaminant concentration as a uniform soil remediation goal could result in relatively small variance in the regional variability of risk. However, for highly mobile and persistent compound like TCE, a single contaminant concentration in soil could result in large variance in the regional variability of risk. For all the contaminants considered, risk varied by orders of magnitude depending in the exposure scenario specified. In all cases, the onsite residential exposure scenario resulted in the greatest risk.

Thus far, of the national and state agencies that have established or proposed uniform soil guidelines, none have considered the regional variability in risk that is likely to result with their use as remediation goals. Rather, uniform goals have been developed using conservative assumptions and deterministic analyses leading some to the conclusion that the uniform approach is inherently conservative and unworkable. Chapter Four, *Establishing and Evaluating the Risk Implications of Uniform Soil Remediation Goals*, examines alternative approaches for establishing uniform soil remediation goals and their risk

implications in light of the methodology and results presented in Chapter Three. Chapter Four describes the use of the methodology in: (1) establishing uniform soil remediation goals to meet a target risk at a specified level of confidence, and (2) evaluating the variability in risk at the uniform soil goal specified. Where the variability in the risk is shown to be large, the possibility of decreasing it by tailoring the uniform goals based on geographical location and limited site information is suggested. This points to the fact that one need not consider the uniform and the site-specific approaches as mutually exclusive. Rather, the two approaches can be thought of as lying on a continuum with a purely site-specific approach on one end and purely uniform approach on the other.

For some contaminants and exposure scenarios (e.g. TCE and the exposure scenarios considered here), a hybrid approach appears best. This would reduce the variance in the regional risk distribution that results from application of a pure uniform approach where a single contaminant concentration is specified for use at all sites. To further reduce the variance, one could add more dimensions to the site categorization scheme until the variance in the risk distribution is acceptable or it is apparent that further reductions in the variance are not possible or worthwhile due to uncertainty in site specific parameter values. SoilRisk and the methodology for evaluating regional risk variability developed here allows consideration and evaluation of such alternatives. Investigation of such hybrid schemes comprises one of the major recommendations for future research made in Chapter 5.

Chapters 1-4
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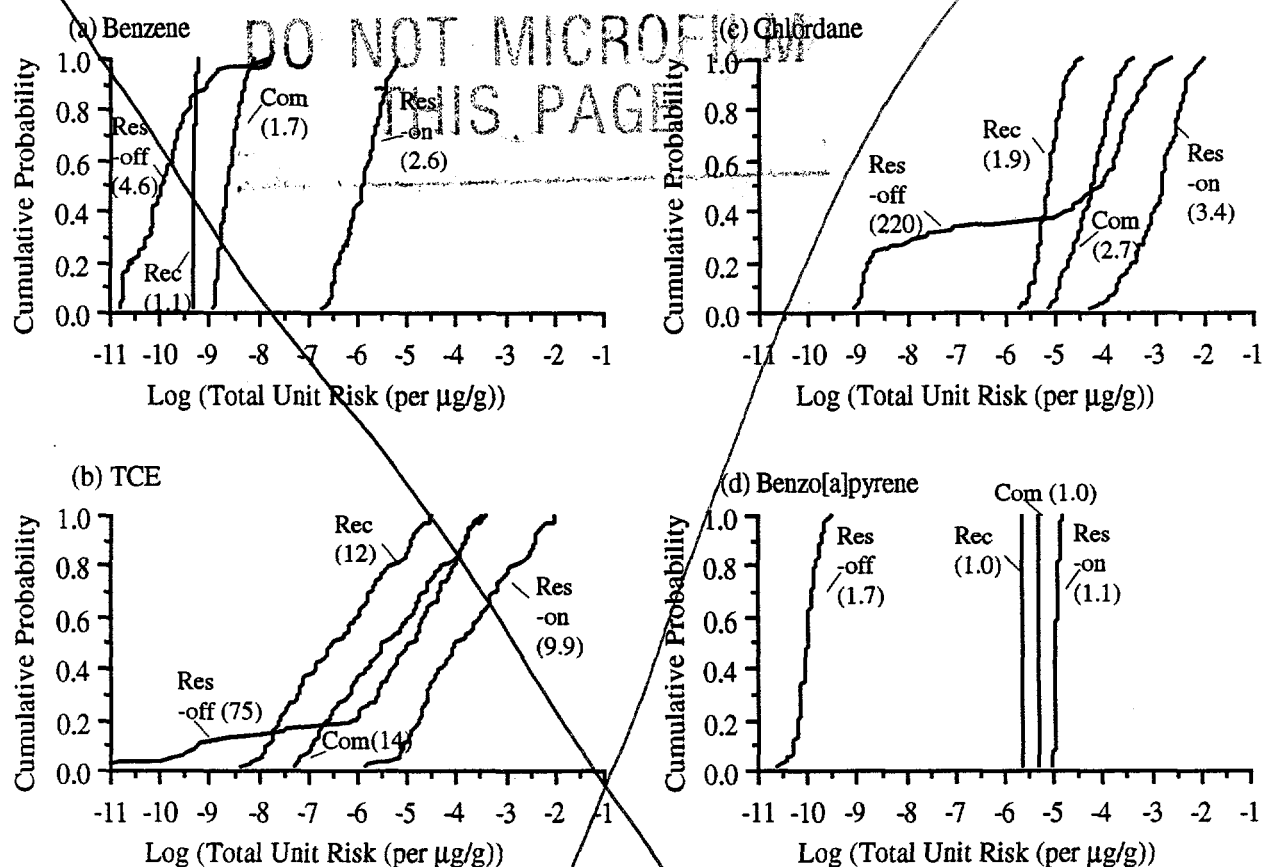


Figure 2: Preliminary total unit risk CDFs for state of Ohio. Geometric standard deviations are given in parentheses. Res-on=residential onsite, Res-off=residential offsite (100m), Rec=recreational, and Com=commercial/industrial. From Labieniec et al. (1994c).

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CHAPTER FIVE:
SUMMARY, CONCLUSIONS,
AND
RECOMMENDATIONS FOR FUTURE RESEARCH

SUMMARY

There has been much debate about how best to establish soil remediation goals at hazardous waste contaminated sites. Yet, quantitative information regarding the risk implications of alternative approaches has been lacking. This research was conducted to develop and demonstrate quantitative tools for evaluating the risk implications of both site-specific and uniform-concentration approaches to setting soil remediation goals.

A review of currently available models revealed the lack of any existing models suitable for integrated exposure and risk assessment of contaminated soil sites. SoilRisk was developed to meet this need for carcinogenic organic contaminants and for use in evaluating the risk implications of approaches to establishing soil remediation goals. It enables deterministic and/or stochastic evaluation of the total risk due to the existence of a contaminated layer in the unsaturated zone. SoilRisk accounts for both volatilization and leaching of the contaminant from soil, and estimates the average contaminant concentrations in the air, soil, and ground water over a specified duration of exposure. Thus, total risk due to a number of different exposure routes can be calculated.

A key component of SoilRisk is an analytical model for the fate and transport of organics in unsaturated soil developed by Jury et al.(1983, 1990). In the integrated model developed, chemical losses from the unsaturated zone occur due to first-order degradation (biological or chemical), volatilization at the soil surface, and leaching to the saturated zone. The unsaturated zone module is linked to modules for air dilution/dispersion, saturated zone transport, and dust generation to allow estimation of long-term average air, groundwater, respirable dust, and soil contaminant concentrations at specified points of exposure. Default values for several different exposure scenarios including recreational,

commercial/industrial, and on- and offsite residential were developed based on current U.S. EPA guidance (U.S. EPA, 1989, 1991).

SoilRisk permits estimation of the carcinogenic risk resulting from a specified contaminant concentration in soil for a specified exposure scenario, or the contaminant concentration in soil to meet a specified level of risk can be determined. These model outputs can be evaluated as single values or as probability distributions, depending on whether site input parameters are specified deterministically or probabilistically. When the model is run probabilistically for a specified exposure scenario, exposure parameters and carcinogenic potency slope factors are treated deterministically. When run in deterministic mode, details of predicted contaminant fate and transport in the subsurface (e.g., contaminant concentration over time and depth below the surface in the unsaturated zone and cumulative mass lost due to volatilization, degradation, and leaching over time) can be obtained.

The key features of SoilRisk include modest input parameter requirements, reflecting typical data availability, and analytical solutions to the environmental fate and transport components of the model, contributing to its computational efficiency.

SoilRisk was applied to evaluate the site-specific and uniform approaches to establishing soil remediation goals at hazardous waste contaminated sites. The uncertainty in the carcinogenic risk estimate due to uncertainty in site conditions at a representative site was quantified in order to evaluate uncertainty in the site-specific approach to setting soil remediation goals. When the uniform approach is considered, variability in risk from site-to-site can occur due to differences in site characteristics that affect transport and fate. To evaluate the variability in the risk estimate across potential sites in a region when a single contaminant concentration in soil is used as a uniform remediation goal, a methodology was developed and applied to a relatively small geographic region for which detailed

hydrogeologic information is available (Ross County, Ohio) and to a relatively larger region (the state of Ohio) for which a full characterization of site variability is not yet possible due to lack of information. Sensitivity of the risk estimate to site parameters was also explored. All analyses performed considered four different suspected or known human carcinogens chosen to represent a wide range of physical/chemical properties (benzene, trichloroethylene (TCE), chlordane, and benzo[a]pyrene (BAP)) and four exposure scenarios (commercial, recreational and on- and offsite residential).

It was shown that the sensitivity of the risk estimate to site conditions varies widely depending on the chemical contaminant and on the exposure scenario specified. As a result, regardless of whether uncertainty in risk at a single site or variability in risk across sites was evaluated, the exposure scenario specified and the properties of the contaminant have more influence on the resulting variance and magnitude of the total risk estimate than variance in site parameters. In general, variance in risk due to variability or uncertainty in site parameters was found to be greater for the relatively less degradable and more mobile of the chemicals studied (TCE and chlordane) than for benzene which is highly degradable and BAP which is very immobile in the subsurface. This difference was attributed to the fact that for the more mobile and persistent compounds, the groundwater exposure routes were predicted to be dominant and saturated zone parameters were found to have a large influence on the risk estimate. The risk estimate for the offsite residential exposure scenario was particularly sensitive to the saturated zone parameters when TCE- and chlordane-contaminated soil were considered. For all the contaminants considered, risk varied by orders of magnitude depending on the exposure scenario specified. In all cases, the onsite residential exposure scenario resulted in the greatest risk.

The methodology for evaluating the uniform-concentration approach in terms of risk variability across sites was demonstrated for use: (1) in establishing uniform soil

remediation goals to meet a target risk at a specified level of confidence, and (2) in evaluating the variability in risk at the uniform soil goal specified.

CONCLUSIONS

From the results, it was concluded that for all contaminants soil remediation goals should be established with consideration of the exposure scenario. For contaminants that are highly degradable such as benzene or immobile in the subsurface such as BAP, specifying a single contaminant concentration for a given exposure scenario as a uniform soil remediation goal can result in relatively small variance in the regional variability of risk. However, for mobile and persistent compound like TCE and chlordane, a single contaminant concentration in soil for a given exposure scenario can result in large variance in the regional variability of risk. For such mobile and persistent compounds, a hybrid approach to setting soil remediation goals is proposed that involves the use of selected site characteristics to identify appropriate soil quality goals from a matrix of acceptable concentration levels. This would reduce the variance in the regional risk distribution that results from application of a pure uniform approach where a single contaminant concentration is specified for use at all sites. To further reduce the variance, one could add more dimensions to the site categorization matrix until the variance in the risk distribution is acceptable or it is apparent that further reductions in the variance are not possible or worthwhile due to uncertainty in site specific parameter values. SoilRisk and the methodology for evaluating regional risk variability developed here allows consideration and evaluation of such alternatives.

RECOMMENDATIONS FOR FUTURE RESEARCH

Many questions and issues remain regarding approaches to establishing soil remediation goals and there are many opportunities for future research. Issues that need to be addressed that came to light as a result of this research are summarized below.

No matter whether a site-specific or a uniform approach is taken to establish soil remediation goals, a quantitative risk assessment model is needed to evaluate the total risk as a function of contaminant concentration in soil. SoilRisk was developed for this purpose, but it has several limitations. The current version of SoilRisk does not account for the existence of a non-aqueous phase liquid (NAPL) and is thus applicable only when the contaminant concentration in soil is less than the theoretical maximum without NAPL as determined by the aqueous solubility, the saturated soil-gas concentration, and the sorptive capacity of the soil. To allow estimation of risk at contaminant concentrations in soil greater than the theoretical maximum, alternative versions of the fate and transport portions of SoilRisk would have to be developed. Several attempts were made to do this while maintaining an analytical solution to the unsaturated zone module, but all involved the assumption of equilibrium dissolution of NAPL. As a result, none provided plausible results. Consideration of NAPL dissolution kinetics is necessary and this would require a numerical model. Also, the current version of SoilRisk is applicable only to organic contaminants in soil. There is a need for similar models for important metal contaminants (e.g., lead, chromium, and mercury).

Additionally, there is a need for experimental and field verification of the fate and transport portions of the current version of SoilRisk as is the case for most other fate and transport models being used or considered for use in risk assessment of contaminated sites.

To enable evaluation of the variability in risk with the use of a uniform-concentration approach to setting soil remediation goals, there is a need for centralized databases describing the variability in site physical/chemical conditions for geographical areas larger than a county or even a state. DRASTIC maps were found to be useful in supplying information regarding the variability in site hydrogeology. However, although these maps

are in the process of being developed for several states, maps are currently only available at the county level. Information to develop site parameter distributions to allow a regional risk assessment of the entire U.S would be required to evaluate the variability in risk due to national uniform soil remediation goals.

This work demonstrated the extreme sensitivity of the risk estimated by SoilRisk to the exposure scenario specified. Throughout the work the exposure assumptions made for each exposure scenario were treated deterministically. Thus, the contribution of variability or uncertainty in exposure conditions to variability or uncertainty in risk for a given exposure scenario was not evaluated. It would be interesting to evaluate the sensitivity of the risk estimate to individual exposure assumptions and, thereby, identify the critical exposure assumptions for each exposure scenario. This could lead to identification of potential institutional controls that would be most effective in reducing risk (e.g. increased buffer distances to site boundaries).

One need not consider the site-specific and uniform approaches to setting soil remediation goals to be mutually exclusive. A hybrid approach was proposed above where sites would be categorized based on limited site information and a matrix of soil remediation goals would be developed for each category. This could reduce the regional variability in risk that can occur with use of a pure uniform-concentration approach where a single contaminant concentration is used as the goal at all sites in a region. There is a need for more research into the influence that alternative site categorization matrices would have on risk variability. Research is needed to identify the maximum reduction in risk variability possible given uncertainty about the conditions at any site and to identify the site categorization matrix that would result in an acceptable level of risk variability with the least amount of site information.

In addition to the evaluation of risk variability, identifying the most advantageous categorization of sites requires an investigation into the economics of the tradeoffs associated with alternative categorization schemes. For example, though additional site information may allow a reduction in risk variability, there are costs associated with obtaining it, including costs of site investigation and regulatory oversight. As alternatives for tailoring the uniform approach to consider more and more site-specific information are proposed, there will be a need for quantitative methodologies for evaluating the economic tradeoffs associated with considering additional site information.

Lastly, no matter what approach is used to establish concentration-based soil remediation goals -- site-specific, uniform-concentration, or some hybrid -- the issue of how to specify the contaminant concentration to be achieved in remediation needs to be addressed. In current practice, soil remediation goals usually are specified deterministically. Statistical criteria are needed to define attainment of a remediation goal specified as a contaminant concentration in soil. For example, the mean and variance of the contaminant concentration to be achieved in remediation or the contaminant concentration along with a level of confidence could be specified. The implications of alternative statistical criteria should be investigated.

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APPENDIX A:
REVIEW OF EXISTING MODELS FOR EXPOSURE
ASSESSMENT OF CONTAMINATED SOIL

INTRODUCTION

Currently, very few models are available that meet the needs for integrated risk assessment at hazardous waste sites with contaminated soil. U.S. EPA guidance on performing exposure and risk assessments at Superfund sites provides information about models available for predicting volatilization from contaminated soil and transport of a contaminant once it enters the air or groundwater (U.S. EPA, 1988, 1989). Guidance on predicting mass leaching rates from contaminated soil is lacking, however, and no single model is given in the guidance for predicting volatilization and leaching simultaneously. To determine which models are being used and how remediation goals are being established at actual sites, the Records of Decision (ROD) and Remedial Investigation/Feasibility Studies were reviewed for 21 Superfund sites in U.S. EPA Regions 1, 2, 3, and 5. (See Appendix F.) It was found that soil cleanup goals have typically been set based on the evaluation of the groundwater ingestion exposure route alone. To this point, the fate and transport models that have been used to assess risk for organic contaminants have only provided estimates of contaminant concentration in groundwater due to leaching; none provided estimates of volatilization.

MODEL REVIEW

The key characteristics of models that have been used or considered appropriate for use in setting soil remediation goals are summarized in Table A-1. Two of the models, the Multimedia Exposure Assessment Model (MULTIMED) (Salhotra et al., 1990, Tsiamos, 1992) and the Multimedia Contaminant Fate, Transport and Exposure Model (MMSOILS) (U.S. EPA, 1992; Root et al., 1991), were developed for use at hazardous waste disposal facilities and provide volatilization emission estimates and modules to predict exposure due to a number of exposure routes. However, neither considers the change in contaminant

concentration in soil over time, and both require the user to input the leaching profile. Thus, neither explicitly models the production of leachate from contaminated soil over time.

The Multimedia Environmental Pollutant Assessment System (MEPAS) is similar to MMSOILS in that it integrates fate and transport and exposure modules to predict risk at hazardous waste disposal facilities and includes a large number of exposure scenarios. MEPAS includes independent modules to predict leaching and volatilization under various circumstances, but does not explicitly model the contaminant concentration profile in the soil as mass is lost over time (Whelan et al., 1992).

The Seasonal Soil Compartment Model (SESOIL) is being considered for use by several states to set soil cleanup goals to meet maximum contaminant concentration levels in groundwater (Hetrick, 1993). It is also being adapted by the American Petroleum Institute for use at petroleum contaminated sites (Bauman, 1992). SESOIL is a compartment model where the soil is divided up into as many as 40 layers and a mass balance is applied to each. Each compartment can lose mass due to both volatilization to the layer above and leaching to the layer below. The mass balance equations applied to each layer are solved simultaneously following each discrete time step. Thus, the SESOIL model is capable of predicting both volatilization and leaching (Bounazountas and Wagner, 1984). However, it has several limitations. The model was initially developed to simulate the fate and transport of a contaminant following its direct application on the soil surface. It can be forced to model the loss of contaminant from an initially contaminated unsaturated zone only by specifying a mass input to each layer in the early time steps. Also, implementation is hampered by the large number of input parameters, some of which are ill defined. In addition, extensive calibration is required (Calabrese et al., 1992).

The Soil-Gas Emission and Leachate Generation (SGELG) model (Nair et al., 1990) simulates the transport of a contaminant from a contaminated layer in the vadose zone and predicts simultaneously the emission rate of a contaminant at the surface and the leach rate at the water table. Of the models reviewed, it is likely the most appropriate model for predicting both volatilization and leaching from an initially contaminated unsaturated zone. A limitation is that it requires a numerical solution which can be time consuming particularly if run stochastically. Also, neither SESOIL nor SGELG are integrated with groundwater transport models, air dilution, dispersion models, nor exposure and risk models.

SUMMARY

To summarize, two models reviewed, MMSOILS and MEPAS, represent fully integrated exposure models, but as indicated in Table 1, they lack the capability to model the loss of contaminant mass from an initially contaminated unsaturated zone. Rather the transport of contaminant mass entering the unsaturated zone from a surface source is modeled which is also true for MULTIMED. Furthermore, the methods used by these three models to predict volatilization rates are not related via mass balance to the leaching estimates. SESOIL and SGELG are strictly unsaturated zone transport models; they are not integrated with other models to allow exposure or risk estimations. Both do allow an initially contaminated unsaturated zone and simulate volatilization, leaching and degradation simultaneously. However, both employ fairly computationally intensive solution techniques. Additionally, SESOIL models 40 soil layers and has fairly intensive input requirements.

Overall, the review of models for organic contaminant fate and transport in the unsaturated zone indicated that available integrated models do not permit simultaneous consideration of volatilization and leaching from a finite zone of initial contamination. The models potentially useful for this purpose involve numerical solutions which would be

computationally expensive and have significant data requirements. With the limited data available to describe most field situations and the long-term predictions required by a carcinogenic risk assessment, a computationally efficient analytical model with a minimum of data requirements was deemed to be more appropriate than computationally burdensome, detailed numerical model with extensive data requirements.

Table A-1: Summary of existing models for exposure assessment for contaminated soils

Characteristic	MULTI-MED	MM-SOILS	MEPAS	SESOIL	SGELG
Unsaturated zone model:					
Initial contamination	No ⁽¹⁾	No ⁽¹⁾	No ⁽¹⁾	Optional ⁽²⁾	Yes ⁽³⁾
Temporal concentration profile	No	No	No	Yes	Yes
Volatilization	Yes	Yes	Yes	Yes	Yes
Leaching	No ⁽⁸⁾	No ⁽⁸⁾	Yes	Yes	Yes
Degradation	Yes	Yes	Yes	Yes	Yes
Type of sol'n.	Semi-an. ⁽⁴⁾	Semi-an. ⁽⁴⁾	Semi-an. ⁽⁴⁾	Iter. ⁽⁵⁾	Num. ⁽⁶⁾
Links to other models:					
Groundwater	Yes	Yes	Yes	No	No
Air dispersion	Yes	Yes	Yes	No	No
Exposure/ Risk	No	Yes	Yes	No	No
Stochastic Capability	Yes	No	No	Yes	No
Source	Salhotra et al.(1990)	U.S.EPA (1992)	Whelan et al.(1992)	Bonazountas and Wagner (1984)	Nair et al. (1990)

Notes: 1. Surface loading specified by user. 2. Surface loading or initial contaminant concentration profile specified by user. 3. Specify an initial contaminant concentration. 4. Semi-an.=Analytical and semi-analytical solution to differential equations. 5. Iter.= Iterative solution to compartmental mass balance at each time step. 6. Num.=Numerical solution to differential equations using a combined finite element/finite difference scheme. 7. An.=Analytical solution to differential equations. 8. Leaching profile specified by user.

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APPENDIX B:
SOILRISK: DETAILED EQUATIONS FOR THE
UNSATURATED ZONE SOLUTE FATE/TRANSPORT
MODULE

Appendix B presents the detailed equations required for the unsaturated zone module in SoilRisk, the integrated soil risk model described in Chapter 1. In cases where original derivations were performed, the derivations are presented.

THE SPACE DERIVATIVE OF C_T , $\frac{\partial C_T(z,t)}{\partial z}$

The space derivative of the total contaminant concentration in soil in the unsaturated zone, $C_T(z,t)$ (Ch. 1, Eq. 1 and Jury (1990, Eq. 17)), was derived by Streile (1988) and checked by the author using Mathematica (Wolfram Research, Inc, 1989):

$$\begin{aligned} \frac{\partial C_T(z,t)}{\partial z} = & \frac{C'_{T0}\rho_b \exp(-\mu t)}{2} \cdot \\ & \left\{ -\frac{1}{\sqrt{\pi D_E t}} \left[\exp\left(-\frac{(z - V_E t - W)^2}{4 D_E t}\right) - \exp\left(-\frac{W V_E}{D_E} - \frac{(z - V_E t + W)^2}{4 D_E t}\right) \right] \right. \\ & \frac{V_E(V_E + H_E)}{H_E D_E} \exp\left(\frac{V_E z}{D_E}\right) \cdot \left(\operatorname{erfc}\left[\frac{(z + V_E t + W)}{2\sqrt{D_E t}}\right] - \operatorname{erfc}\left[\frac{(z + V_E t)}{2\sqrt{D_E t}}\right] \right) + \\ & \frac{(V_E + 2H_E)(V_E + H_E)}{H_E D_E} \cdot \exp\left(\frac{(V_E + H_E)(z + H_E t)}{D_E}\right) \cdot \\ & \left. \left(\operatorname{erfc}\left[\frac{(z + (V_E + 2H_E)t)}{2\sqrt{D_E t}}\right] - \exp\left(\frac{H_E W}{D_E}\right) \operatorname{erfc}\left[\frac{(z + (V_E + 2H_E)t + W)}{2\sqrt{D_E t}}\right] \right) \right\} \end{aligned} \quad (B-1)$$

where:

$$\mu = \frac{\ln(2)}{\tau} \quad = \text{effective first order reaction rate constant (d}^{-1}\text{)}, \quad (B-2)$$

$$V_E = \frac{J_w}{K_T} \quad = \text{effective solute velocity (m/day)}, \quad (B-3)$$

$$D_E = \frac{\left(a^{10/3} D_g^a K_H + \theta^{10/3} D_l^w\right)}{\eta^2 K_T} \quad = \text{effective diffusion coefficient (m}^2\text{/day)}, \quad (B-4)$$

$$K_T = \rho_b f_{oc} K_{oc} + \theta + a K_H \quad = \text{equilibrium distribution coefficient between total and aqueous phase contaminant concentrations (-)}, (B-5)$$

$$H_E = \frac{D_g^a K_H}{K_T d} \quad (B-6)$$

and C'_{T0} ($\mu\text{g/g}$) is the initial total contaminant concentration in the contaminated layer, ρ_b (g/cm^3) is the soil bulk density, z (m) is the depth below the soil surface, t (day) is time, W

(m) is the thickness of the contaminated layer, τ (day) is the effective half-life of the contaminant in soil, J_w (m/day) is the soil-water volumetric flux rate, a is the volumetric air content of the soil equal to $(\eta - \theta)$, θ is the volumetric soil water content, η is the soil porosity, D_g^a (m²/day) is the gaseous diffusion coefficient of the contaminant in air, D_l^w (m²/day) is the liquid diffusion coefficient of the contaminant in water, K_H is the dimensionless Henry's Law coefficient, f_{oc} is the fraction organic carbon in soil, K_{oc} (cm³/g) is the equilibrium partition coefficient normalized to organic C, and d (m) is the soil-atmosphere boundary layer thickness.

THE INTEGRAL OVER TIME OF C_T , $\int_0^t C_T(z, t') dt'$

The equation for $\int_0^t C_T(z, t') dt'$ was derived analytically by noting that $C_T(z, t)$ can be re-

written as a constant times the sum of 6 terms:

$$C_T(z, t) = \frac{C'_{T0}\rho_b}{2} \sum_{j=1}^6 c_j \cdot f_j(t) \quad (B-7)$$

in which case:

$$\int_0^t C_T(z, t') dt' = \frac{C'_{T0}\rho_b}{2} \sum_{j=1}^6 \left(c_j \cdot \int_0^t f_j(t') dt' \right) \quad (B-8)$$

where:

$$c_1 = 1$$

$$c_2 = -1$$

$$c_3 = \left(1 + \frac{V_E}{H_E} \right) \exp \left[\frac{V_E z}{D_E} \right]$$

$$c_4 = - \left(1 + \frac{V_E}{H_E} \right) \exp \left[\frac{V_E z}{D_E} \right]$$

$$c_5 = \left(2 + \frac{V_E}{H_E} \right) \exp \left[\frac{(H_E + V_E)z}{D_E} \right]$$

$$c_6 = - \left(2 + \frac{V_E}{H_E} \right) \exp \left[\frac{(H_E + V_E)z}{D_E} + \frac{H_E W}{D_E} \right]$$

and the general form of $f_j(t)$ is:

$$f_j(t) = \exp[(a^2 - \alpha)t] \operatorname{erfc}\left[x \frac{1}{2\sqrt{t}} + a\sqrt{t}\right] \quad (\text{B-9})$$

where f_j , α , a , and x are as shown in Table B-1.

A general formula for $\int_0^t f_j(t') dt'$ was derived using a Laplace transform where:

$$\int_0^t f_j(t') dt' = \mathcal{L}^{-1}\left\{\frac{1}{s} \mathcal{L}\{f_j(t)\}\right\} \quad (\text{B-10})$$

where definition of the Laplace transform is:

$$\mathcal{L}\{f(t)\} = \int_0^\infty \exp[-st] f(t) dt = F(s) \quad (\text{B-11})$$

by following Streile (1988, p.19) and using Erdelyi (1954, p.177, Eq. 12). The general formula derived for $\int_0^t f_j(t') dt'$ is:

$$\begin{aligned} \int_0^t f_j(t') dt' = & -\frac{\exp[-t(\alpha - a^2)]}{(\alpha - a^2)} \operatorname{erfc}\left[\frac{x}{2\sqrt{t}} + a\sqrt{t}\right] + \\ & \frac{\exp[-ax + x\sqrt{\alpha}]}{2(\alpha - a^2)} \operatorname{erfc}\left[\frac{x}{2\sqrt{t}} - \sqrt{\alpha t}\right] \left(1 - \frac{a}{\sqrt{\alpha}}\right) + \\ & \frac{\exp[-ax + x\sqrt{\alpha}]}{2(\alpha - a^2)} \operatorname{erfc}\left[\frac{x}{2\sqrt{t}} + \sqrt{\alpha t}\right] \left(1 + \frac{a}{\sqrt{\alpha}}\right) \quad \text{for } x \geq 0 \end{aligned} \quad (\text{B-12})$$

Table B-1: Equations for f_i and identification of α , a , and x

Equation for f_i †	α (day ⁻¹)	a (day ^{-1/2})	x (day ^{1/2})	$(\alpha-a^2)$ (day ⁻¹)
$f_1 = \exp[-\mu t] \operatorname{erfc} \left[\frac{z - W - V_E t}{2\sqrt{D_E t}} \right]$ for $z \geq W$	β^2	$-\frac{V_E}{\sqrt{4D_E}}$	$\frac{z - W}{\sqrt{D_E}}$	μ
$f_2 = \exp[-\mu t] \operatorname{erfc} \left[\frac{z - V_E t}{2\sqrt{D_E t}} \right]$	β^2	$-\frac{V_E}{\sqrt{4D_E}}$	$\frac{z}{\sqrt{D_E}}$	μ
$f_3 = \exp[-\mu t] \operatorname{erfc} \left[\frac{z + W + V_E t}{2\sqrt{D_E t}} \right]$	β^2	$\frac{V_E}{\sqrt{4D_E}}$	$\frac{z + W}{\sqrt{D_E}}$	μ
$f_4 = \exp[-\mu t] \operatorname{erfc} \left[\frac{z + V_E t}{2\sqrt{D_E t}} \right]$	β^2	$\frac{V_E}{\sqrt{4D_E}}$	$\frac{z}{\sqrt{D_E}}$	μ
$f_5 = \exp[(\xi - \mu)t] \operatorname{erfc} \left[\frac{z + (2H_E + V_E)t}{2\sqrt{D_E t}} \right]$	β^2	$\frac{2H_E + V_E}{\sqrt{4D_E}}$	$\frac{z}{\sqrt{D_E}}$	$\mu - \xi$
$f_6 = \exp[(\xi - \mu)t] \operatorname{erfc} \left[\frac{z + W + (2H_E + V_E)t}{2\sqrt{D_E t}} \right]$	β^2	$\frac{2H_E + V_E}{\sqrt{4D_E}}$	$\frac{z + W}{\sqrt{D_E}}$	$\mu - \xi$

† where $\xi = (H_E + V_E)H_E/D_E$. and $\beta = \sqrt{V_E^2/4D_E + \mu}$.

When α , a , x , and $(\alpha-a^2)$ as presented in Table B-1 are assigned to Eq. B-12 to get the time integral of f_1 :

$$\begin{aligned}
 \left[c_1 \int_0^t f_1(t') dt' \right]_{\text{for } z \geq W} &= -\frac{1}{\mu} \exp[-\mu t] \operatorname{erfc} \left[\frac{z - W - V_E t}{2\sqrt{D_E t}} \right] + \\
 &\frac{1}{2\mu} \exp \left[\frac{V_E z}{2D_E} - \frac{P}{2} - \frac{\beta(z - W)}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z - W}{2\sqrt{D_E t}} - \beta\sqrt{t} \right] \left(1 + \frac{V_E}{2\beta\sqrt{D_E}} \right) + \\
 &\frac{1}{2\mu} \exp \left[\frac{V_E z}{2D_E} - \frac{P}{2} + \frac{\beta(z - W)}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z - W}{2\sqrt{D_E t}} + \beta\sqrt{t} \right] \left(1 - \frac{V_E}{2\beta\sqrt{D_E}} \right)
 \end{aligned} \tag{B-13a}$$

Eq. B-13a is for the case when $z \geq W$ because the general formula in Eq. B-12 is for the case when $x \geq 0$. For $z < W$, the rule $\operatorname{erfc}(-x) = 2 - \operatorname{erfc}(x)$ is applied to f_1 which, when rearranged, looks like:

$$f_1 = 2 \exp[-\mu t] - \exp[-\mu t] \operatorname{erfc} \left[\frac{-(z-W) + V_E t}{2\sqrt{D_E t}} \right]$$

The second term conforms the general form of f_j given in Eq. B-9 where

$\alpha = V_E^2/(4D_E) + \mu$, $a = V_E/\sqrt{4D_E}$, and $x = -(z-W)/\sqrt{4D_E}$. By integrating the first term directly, applying the general formula given in Eq. B-12 to obtain the integral of the second term, and re-arranging:

$$\begin{aligned} \left[c_1 \int_0^t f_1(t') dt' \right]_{\text{for } z < W} &= \left[c_1 \int_0^t f_1(t') dt' \right]_{\text{for } z \geq W} + \frac{2}{\mu} \\ &\quad - \frac{1}{\mu} \exp \left[\frac{V_E z}{2D_E} - \frac{P}{2} - \frac{\beta(z-W)}{\sqrt{D_E}} \right] \left(1 + \frac{V_E}{2\beta\sqrt{D_E}} \right) - \\ &\quad \frac{1}{\mu} \exp \left[\frac{V_E z}{2D_E} - \frac{P}{2} + \frac{\beta(z-W)}{\sqrt{D_E}} \right] \left(1 - \frac{V_E}{2\beta\sqrt{D_E}} \right) \end{aligned} \quad (\text{B-13b})$$

When α , a , x , and (αa^2) as presented in Table B-1 are assigned to Eq. B-12 to get the time integral of f_2 through f_6 :

$$\begin{aligned} c_2 \int_0^t f_2(t') dt' &= \frac{1}{\mu} \exp[-\mu t] \operatorname{erfc} \left[\frac{z - V_E t}{2\sqrt{D_E t}} \right] - \\ &\quad \frac{1}{2\mu} \exp \left[\frac{V_E z}{2D_E} - \frac{z\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z}{2\sqrt{D_E t}} - \beta\sqrt{t} \right] \left(1 + \frac{V_E}{2\beta\sqrt{D_E}} \right) - \\ &\quad \frac{1}{2\mu} \exp \left[\frac{V_E z}{2D_E} + \frac{z\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z}{2\sqrt{D_E t}} + \beta\sqrt{t} \right] \left(1 - \frac{V_E}{2\beta\sqrt{D_E}} \right) \end{aligned} \quad (\text{B-14})$$

$$\begin{aligned} c_3 \int_0^t f_3(t') dt' &= \left(1 + \frac{V_E}{H_E} \right) \left\{ -\frac{1}{\mu} \exp \left[-\mu t + \frac{V_E z}{D_E} \right] \operatorname{erfc} \left[\frac{z+W+V_E t}{2\sqrt{D_E t}} \right] + \right. \\ &\quad \frac{1}{2\mu} \exp \left[\frac{V_E z}{2D_E} - \frac{P}{2} - \frac{(z+W)\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z+W}{2\sqrt{D_E t}} - \beta\sqrt{t} \right] \left(1 - \frac{V_E}{2\beta\sqrt{D_E}} \right) + \\ &\quad \left. \frac{1}{2\mu} \exp \left[\frac{V_E z}{2D_E} - \frac{P}{2} + \frac{(z+W)\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z+W}{2\sqrt{D_E t}} + \beta\sqrt{t} \right] \left(1 + \frac{V_E}{2\beta\sqrt{D_E}} \right) \right\} \end{aligned} \quad (\text{B-15})$$

$$\begin{aligned}
c_4 \int_0^t f_4(t') dt' = & - \left(1 + \frac{V_E}{H_E} \right) \left\{ - \frac{1}{\mu} \exp \left[-\mu t + \frac{V_E z}{D_E} \right] \operatorname{erfc} \left[\frac{z + V_E t}{2\sqrt{D_E t}} \right] + \right. \\
& \frac{1}{2\mu} \exp \left[\frac{V_E z}{2D_E} - \frac{z\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z}{2\sqrt{D_E t}} - \beta\sqrt{t} \right] \left(1 - \frac{V_E}{2\beta\sqrt{D_E}} \right) + \\
& \left. \frac{1}{2\mu} \exp \left[\frac{V_E z}{2D_E} + \frac{z\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z}{2\sqrt{D_E t}} + \beta\sqrt{t} \right] \left(1 + \frac{V_E}{2\beta\sqrt{D_E}} \right) \right\}
\end{aligned} \quad (\text{B-16})$$

$$\begin{aligned}
c_5 \int_0^t f_5(t') dt' = & \left(2 + \frac{V_E}{H_E} \right) \cdot \\
& \left\{ - \frac{1}{(\mu - \xi)} \exp \left[-(\mu - \xi)t + \frac{H_E z}{D_E} + \frac{V_E z}{D_E} \right] \operatorname{erfc} \left[\frac{z + (V_E + 2H_E)t}{2\sqrt{D_E t}} \right] + \right. \\
& \frac{1}{2(\mu - \xi)} \exp \left[\frac{V_E z}{2D_E} - \frac{z\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z}{2\sqrt{D_E t}} - \beta\sqrt{t} \right] \left(1 - \frac{(V_E + 2H_E)}{2\beta\sqrt{D_E}} \right) + \\
& \left. \frac{1}{2(\mu - \xi)} \exp \left[\frac{V_E z}{2D_E} + \frac{z\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z}{2\sqrt{D_E t}} + \beta\sqrt{t} \right] \left(1 + \frac{(V_E + 2H_E)}{2\beta\sqrt{D_E}} \right) \right\}
\end{aligned} \quad (\text{B-17})$$

$$\begin{aligned}
c_6 \int_0^t f_6(t') dt' = & \left(2 + \frac{V_E}{H_E} \right) \cdot \\
& \left\{ \frac{1}{(\mu - \xi)} \exp \left[\frac{H_E z}{D_E} + \frac{V_E z}{2D_E} + \frac{H_E W}{D_E} - (\mu - \xi)t \right] \operatorname{erfc} \left[\frac{z + W + (V_E + 2H_E)t}{2\sqrt{D_E t}} \right] - \right. \\
& \frac{1}{2(\mu - \xi)} \exp \left[\frac{V_E z}{2D_E} - \frac{P}{2} - \frac{(z + W)\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z + W}{2\sqrt{D_E t}} - \beta\sqrt{t} \right] \left(1 - \frac{(V_E + 2H_E)}{2\beta\sqrt{D_E}} \right) - \\
& \left. \frac{1}{2(\mu - \xi)} \exp \left[\frac{V_E z}{2D_E} - \frac{P}{2} + \frac{(z + W)\beta}{\sqrt{D_E}} \right] \operatorname{erfc} \left[\frac{z + W}{2\sqrt{D_E t}} + \beta\sqrt{t} \right] \left(1 + \frac{(V_E + 2H_E)}{2\beta\sqrt{D_E}} \right) \right\}
\end{aligned} \quad (\text{B-18})$$

where $\xi = (H_E + V_E)H_E/D_E$, $P = V_E W/D_E$, $\beta = \sqrt{V_E^2/(4D_E) + \mu}$.

The integrals for f_j were all checked using Mathematica (Wolfram Research, Inc., 1989) by ensuring that $\frac{d}{dt} \left[\int_0^t f_j(t') dt' \right] = f_j(t)$.

THE INTEGRAL OVER TIME OF THE SPACE DERIVATIVE OF C_T ,

$$\int_0^t \frac{\partial C_T(z, t')}{\partial z} dt'$$

The equation for $\int_0^t \frac{\partial C_T(z, t')}{\partial z} dt'$ was derived by noting that:

$$\int_0^t \frac{\partial C_T(z, t')}{\partial z} dt' = \frac{\partial}{\partial z} \int_0^t C_T(z, t') dt' = \frac{C'_{T0} \rho_b}{2} \sum_{j=1}^6 \left(c_j \cdot \frac{\partial}{\partial z} \int_0^t f_j(t') dt' \right) \quad (\text{B-19})$$

With the aid of Mathematica (Wolfram Research, Inc., 1989), equations for $\frac{\partial}{\partial z} \int_0^t f_j(t') dt'$ were derived, combined according to Eq. B-19, and simplified:

$$\begin{aligned} \left[\int_0^t \frac{\partial C_T(z, t')}{\partial z} dt' \right]_{z \geq W} &= \frac{C'_{T0} \rho_b}{2} \left\{ \left(1 + \frac{V_E}{H_E} \right) \frac{V_E}{\mu D_E} \exp[-\mu t] (S_{5a} - S_{4a}) + \right. \\ &\quad \left(2 + \frac{V_E}{H_E} \right) \left(\frac{H_E}{D_E} + \frac{V_E}{D_E} \right) \left(\frac{1}{\mu - \xi} \right) \exp[-(\mu - \xi)t] (S_{7a} - S_{6a}) + \\ &\quad \frac{1}{2\beta\sqrt{D_E}} \exp\left[\frac{V_E z}{2D_E} \right] \left\{ \exp\left[-\frac{P}{2} \right] (S_{1b} - S_{1a}) + S_{3a} - S_{3b} \right\} + \\ &\quad \left(1 + \frac{V_E}{H_E} \right) \left(\frac{1}{2\mu} \right) \exp\left[\frac{V_E z}{2D_E} \right] \cdot \\ &\quad \left\{ \exp\left[-\frac{P}{2} \right] (R_{1a} S_{2a} + R_{1b} S_{2b}) - R_{1a} S_{3a} - R_{1b} S_{3b} \right\} + \\ &\quad \left(2 + \frac{V_E}{H_E} \right) \left(\frac{1}{2(\mu - \xi)} \right) \exp\left[\frac{V_E z}{2D_E} \right] \cdot \\ &\quad \left\{ R_{2a} S_{3a} + R_{2b} S_{3b} - \exp\left[-\frac{P}{2} \right] (R_{2a} S_{2a} + R_{2b} S_{2b}) \right\} \end{aligned} \quad (\text{B-20a})$$

$$\begin{aligned} \left[\int_0^t \frac{\partial C_T(z, t')}{\partial z} dt' \right]_{\text{for } z < W} &= \left[\int_0^t \frac{\partial C_T(z, t')}{\partial z} dt' \right]_{\text{for } z \geq W} + \\ &\quad \frac{1}{\mu} \left(\frac{\beta}{\sqrt{D_E}} - \frac{V_E^2}{4\beta D_E^{3/2}} \right) \exp\left[-\frac{P}{2} + \frac{V_E z}{2D_E} \right] \left(\exp\left[-\frac{\beta(z-W)}{\sqrt{D_E}} \right] - \exp\left[\frac{\beta(z-W)}{\sqrt{D_E}} \right] \right) \end{aligned} \quad (\text{B-20b})$$

where $\xi = (H_E + V_E)H_E/D_E$, $P = V_E W/D_E$, $\beta = \sqrt{V_E^2/(4D_E) + \mu}$, and

$$S_{1a} = \exp\left[-(z-W)\frac{\beta}{\sqrt{D_E}}\right] \operatorname{erfc}\left[\frac{(z-W)}{2\sqrt{D_E t}} - \beta\sqrt{t}\right]$$

$$S_{1b} = \exp\left[(z-W)\frac{\beta}{\sqrt{D_E}}\right] \operatorname{erfc}\left[\frac{(z-W)}{2\sqrt{D_E t}} + \beta\sqrt{t}\right]$$

$$S_{2a} = \exp\left[-(z+W)\frac{\beta}{\sqrt{D_E}}\right] \operatorname{erfc}\left[\frac{(z+W)}{2\sqrt{D_E t}} - \beta\sqrt{t}\right]$$

$$S_{2b} = \exp\left[(z+W)\frac{\beta}{\sqrt{D_E}}\right] \operatorname{erfc}\left[\frac{(z+W)}{2\sqrt{D_E t}} + \beta\sqrt{t}\right]$$

$$S_{3a} = \exp\left[-z\frac{\beta}{\sqrt{D_E}}\right] \operatorname{erfc}\left[\frac{z}{2\sqrt{D_E t}} - \beta\sqrt{t}\right]$$

$$S_{3b} = \exp\left[z\frac{\beta}{\sqrt{D_E}}\right] \operatorname{erfc}\left[\frac{z}{2\sqrt{D_E t}} + \beta\sqrt{t}\right]$$

$$S_{4a} = \exp\left[\frac{V_E z}{D_E}\right] \operatorname{erfc}\left[\frac{z+W+V_E t}{2\sqrt{D_E t}}\right]$$

$$S_{5a} = \exp\left[\frac{V_E z}{D_E}\right] \operatorname{erfc}\left[\frac{z+V_E t}{2\sqrt{D_E t}}\right]$$

$$S_{6a} = \exp\left[\frac{z(H_E + V_E)}{D_E}\right] \operatorname{erfc}\left[\frac{z+(2H_E + V_E)t}{2\sqrt{D_E t}}\right]$$

$$S_{7a} = \exp\left[\frac{z(H_E + V_E) + H_E W}{D_E}\right] \operatorname{erfc}\left[\frac{W+z+(2H_E + V_E)t}{2\sqrt{D_E t}}\right]$$

$$R_{1a} = \left(1 - \frac{V_E}{2\beta\sqrt{D_E}}\right) \left(\frac{V_E}{2D_E} - \frac{\beta}{\sqrt{D_E}}\right)$$

$$R_{1b} = \left(1 + \frac{V_E}{2\beta\sqrt{D_E}}\right) \left(\frac{V_E}{2D_E} + \frac{\beta}{\sqrt{D_E}}\right)$$

$$R_{2a} = \left(1 - \frac{(V_E + 2H_E)}{2\beta\sqrt{D_E}}\right) \left(\frac{V_E}{2D_E} - \frac{\beta}{\sqrt{D_E}}\right)$$

$$R_{2b} = \left(1 + \frac{(V_E + 2H_E)}{2\beta\sqrt{D_E}}\right) \left(\frac{V_E}{2D_E} + \frac{\beta}{\sqrt{D_E}}\right)$$

THE INTEGRAL OVER SPACE OF C_T , $\int_0^z C_T(z', t) dz'$

An equation for $\int_0^z C_T(z', t) dz'$ was derived by Streile (1988, p.26) and was checked by the

author using Mathematica (Wolfram Research, Inc., 1989) by ensuring that

$\frac{\partial}{\partial z} \int_0^z C_T(z', t) dz' = C_T(z, t)$. Several errors were detected in Streile's original derivation

and are corrected here:

$$\int_0^z C_T(z', t) dz' = \frac{C'_{T0} \rho_b}{2} \exp(-\mu t) (sum_2 - sum_1) \quad (B-21)$$

$$\int_0^\infty C_T(z', t) dz' = \frac{C'_{T0} \rho_b}{2} \exp(-\mu t) (sum_2) \quad (B-22)$$

$$\int_z^\infty C_T(z', t) dz' = -\frac{C'_{T0} \rho_b}{2} \exp(-\mu t) (sum_1) \quad (B-23)$$

where:

$$sum_1 = 2\sqrt{\frac{D_E t}{\pi}} S_8 + (z - V_E t) S_1 - (z - V_E t - W) S_2 + \frac{D_E}{V_E} \left(1 + \frac{V_E}{H_E}\right) (S_3 - S_4 - S_1 + S_5) + \frac{D_E}{(V_E + H_E)} \left(2 + \frac{V_E}{H_E}\right) (S_6 - S_7 - S_5 + S_1) \quad (B-24)$$

where:

$$S_1 = \operatorname{erfc} \left[\frac{z - V_E t}{2\sqrt{D_E t}} \right]$$

$$S_2 = \operatorname{erfc} \left[\frac{z - W - V_E t}{2\sqrt{D_E t}} \right]$$

$$S_3 = \exp \left[\frac{V_E z}{D_E} \right] \operatorname{erfc} \left[\frac{z + V_E t}{2\sqrt{D_E t}} \right]$$

$$S_4 = \exp \left[\frac{V_E z}{D_E} \right] \operatorname{erfc} \left[\frac{z + W + V_E t}{2\sqrt{D_E t}} \right]$$

$$S_5 = \exp[-P] \operatorname{erfc} \left[\frac{z + W - V_E t}{2\sqrt{D_E t}} \right]$$

$$S_6 = \exp \left[\xi t + \frac{(V_E + H_E)z}{D_E} + \frac{H_E W}{D_E} \right] \operatorname{erfc} \left[\frac{z + W + (V_E + 2H_E)t}{2\sqrt{D_E t}} \right]$$

$$S_7 = \exp \left[\xi t + \frac{(V_E + H_E)z}{D_E} \right] \operatorname{erfc} \left[\frac{z + (V_E + 2H_E)t}{2\sqrt{D_E t}} \right]$$

$$S_8 = \exp \left[-\frac{(z - W - V_E t)^2}{4D_E t} \right] - \exp \left[-\frac{(z - V_E t)^2}{4D_E t} \right]$$

and

$$\begin{aligned} \text{sum}_2 = & 2\sqrt{\frac{D_E t}{\pi}} S_8 + (V_E t + W)(1 + S_2) - V_E t(1 + S_1) + \\ & \frac{D_E}{V_E} \left(1 + \frac{V_E}{H_E} \right) (S_2 - S_1 + S_5 - 1 - S_1) + \frac{D_E}{(V_E + H_E)} \left(2 + \frac{V_E}{H_E} \right) (S_4 - S_3 - S_5 + 1 + S_1) \end{aligned}$$

where:

$$S_1 = \operatorname{erf} \left[\frac{V_E t}{2\sqrt{D_E t}} \right]$$

$$S_2 = \operatorname{erf} \left[\frac{V_E t + W}{2\sqrt{D_E t}} \right]$$

$$S_3 = \exp[\xi t] \operatorname{erfc} \left[\frac{(V_E + 2H_E)t}{2\sqrt{D_E t}} \right]$$

$$S_4 = \exp \left[\xi t + \frac{H_E W}{D_E} \right] \operatorname{erfc} \left[\frac{(V_E + 2H_E)t + W}{2\sqrt{D_E t}} \right]$$

$$S_5 = \exp[-P] \operatorname{erfc} \left[\frac{W - V_E t}{2\sqrt{D_E t}} \right]$$

$$S_8 = \exp \left[-\frac{(V_E t + W)^2}{4D_E t} \right] - \exp \left[-\frac{(V_E t)^2}{4D_E t} \right]$$

and $\xi = (H_E + V_E)H_E/D_E$, $P = V_E W/D_E$.

THE CUMULATIVE VOLATILIZATION LOSS FROM THE SOIL

SURFACE, $\int_0^t -J_t(0, t') dt'$

Jury et al. (1990, Eq. A2) and Streile (1988, pp.16-25) provide an equation for the cumulative volatilization loss from the soil surface between times 0 and t for a chemical initially deposited between 0 and W at a concentration of C'_{T0} ($\mu\text{g/g}$). Several

typographical errors were detected in the equation presented by Jury et al. (1990). These are corrected here.

$$\begin{aligned}
 \int_0^t -J_t(0, t'; W) dt' = & -\frac{C_{T0}\rho_b}{2} \left\{ \frac{V_E}{\mu} [1 - \exp(-\mu t)] [S_1 - S_2] - \right. \\
 & \frac{(V_E + 2H_E)}{(\mu - \xi)} \cdot [1 - \exp(-\mu t)] [S_3 - S_4] + \\
 & \exp\left[-\frac{P}{2} - \frac{\beta W}{\sqrt{D_E}}\right] \cdot \left[\frac{(V_E + 2H_E)}{2(\mu - \xi)} - \frac{V_E}{2\mu} - \frac{(V_E + 2H_E)^2}{4(\mu - \xi)\beta\sqrt{D_E}} + \frac{V_E^2}{4\mu\beta\sqrt{D_E}} \right] S_5 + \\
 & \exp\left[-\frac{P}{2} + \frac{\beta W}{\sqrt{D_E}}\right] \cdot \left[\frac{(V_E + 2H_E)}{2(\mu - \xi)} - \frac{V_E}{2\mu} + \frac{(V_E + 2H_E)^2}{4(\mu - \xi)\beta\sqrt{D_E}} - \frac{V_E^2}{4\mu\beta\sqrt{D_E}} \right] S_6 + \\
 & \left. \frac{1}{2\beta\sqrt{D_E}} \left[\frac{(V_E + 2H_E)^2}{(\mu - \xi)} - \frac{V_E^2}{\mu} \right] S_7 \right\} \quad (B-26)
 \end{aligned}$$

where $P = V_E W / D_E$, $\xi = (H_E + V_E) H_E / D_E$, $\beta = \sqrt{V_E^2 / (4D_E) + \mu}$, and

$$S_1 = \operatorname{erfc}\left[\frac{V_E t}{\sqrt{4D_E t}}\right]$$

$$S_2 = \operatorname{erfc}\left[\frac{(W + V_E t)}{\sqrt{4D_E t}}\right]$$

$$S_3 = \exp(\xi t) \operatorname{erfc}\left[\frac{(V_E + 2H_E)t}{\sqrt{4D_E t}}\right]$$

$$S_4 = \exp\left(\xi t + \frac{H_E W}{D_E}\right) \operatorname{erfc}\left[\frac{W + (V_E + 2H_E)t}{\sqrt{4D_E t}}\right]$$

$$S_5 = \operatorname{erfc}\left[\frac{W}{\sqrt{4D_E t}} - \beta\sqrt{t}\right]$$

$$S_6 = \operatorname{erfc}\left[\frac{L}{\sqrt{4D_E t}} + \beta\sqrt{t}\right]$$

$$S_7 = \operatorname{erf}[\beta\sqrt{t}]$$

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APPENDIX C:
SOILRISK: ESTIMATION METHOD FOR COMPOUND
DIFFUSION COEFFICIENTS AND K_H

In the model, the gaseous diffusion coefficient in air, D_g^a , the liquid diffusion coefficient in water, D_l^w , and the dimensionless Henry's coefficient, K_H , are calculated as a function of temperature using the properties summarized in Table C-1 for the various contaminants of interest.

ESTIMATION OF D_g^a

The gaseous diffusion coefficient of the contaminant in air, D_g^a (m^2/day), as a function of temperature, $T(^{\circ}C)$, is estimated using the method of Wilkes and Lee, a method recommended by Lyman et al. (1990, Section 17-4):

$$D_g^a = \frac{B' (T + 273.2)^{1.5} \sqrt{(28.97 + MW)/(28.97 \cdot MW)}}{P \sigma_{AB}^2 \Omega} \cdot 8.64 \quad (C-1)$$

where MW is the molecular weight of the compound of interest, P is pressure in atm and is set equal to one. The parameters, B' , σ_{AB} , and Ω , are defined below:

$$B' = 0.00217 - 0.00050 \sqrt{1/28.97 + 1/MW} \quad (C-2)$$

$$\Omega = \frac{a}{(T^*)^b} + \frac{c}{\exp(T^*d)} + \frac{e}{\exp(T^*f)} + \frac{g}{\exp(T^*h)} \quad (C-3)$$

where,

$a=1.06036$	$c=0.19300$	$e=1.03587$	$g=1.76474$
$b=0.15610$	$d=0.47635$	$f=1.52996$	$h=3.89411$

and,

$$T^* = \frac{T + 273.2}{\sqrt{(78.6 \cdot 1.15(T_b + 273.2))}} \quad (C-4)$$

where T_b is the boiling point of the compound in $^{\circ}C$ and σ_{AB} is defined as:

$$\sigma_{AB} = \frac{3.711 + 1.18(V_B')^{1/3}}{2} \quad (C-5)$$

where V_B' is the LeBas molar volume of the compound of interest in $cm^3/mole$ which can be determined using Table 17-5 in Lyman et al. (1990).

ESTIMATION OF D_l^w

The Hayduk and Laudie method presented in Lyman et al.(1990), Section 17-7, is used to calculate the diffusion coefficient of the chemical of concern in water, D_l^w (m^2/day), as a function of temperature:

$$D_l^w = \frac{13.26 \times 10^{-5}}{\eta_w^{1.14} V_B^{0.589}} \cdot 8.64 \quad (C-6)$$

where η_w is the viscosity of water in centipoise at the temperature of interest. Data for η_w for temperatures ranging from zero to 30°C from Lyman et al.(1990) are provided in the code.

ESTIMATION OF K_H

The algorithm used to adjust the dimensionless Henry's Law coefficient, K_H , as a function of temperature, T , is based on the Claussius-Clayperon equation and consideration of temperature effects on solubility (Dzombak et al., 1993):

$$K_H(T) = \exp \left[\frac{\Delta H_v(T_{KH})}{R(T_{KH} + 273.2)} - \frac{\Delta H_v(T)}{R(T + 273.2)} \right] \cdot K_H(T_{KH}) \quad (C-7)$$

where $K_H(T_{KH})$ is the dimensionless Henry's coefficient at reference temperature, T_{KH} (°C, typically 20 or 25°C), R is the gas constant (1.9872 cal/mol-K), and ΔH_v (cal/mol) is the molar heat of vaporization. ΔH_v is estimated using Eq. 13-21 and Table 13-7 in Lyman et al. (1990):

$$\Delta H_v = \Delta H_{vB} \left[\frac{1 - (T + 273.2)/(T_c + 273.2)}{1 - (T_b + 273.2)/(T_c + 273.2)} \right]^n \quad (C-8)$$

where:

$$n = \begin{cases} 0.30 & \frac{T_b + 273.2}{T_c + 273.2} < 0.57 \\ 0.74 \left(\frac{T_b + 273.2}{T_c + 273.2} \right) - 0.116 & 0.57 \leq \frac{T_b + 273.2}{T_c + 273.2} \leq 0.71 \\ 0.41 & \frac{T_b + 273.2}{T_c + 273.2} < 0.71 \end{cases} \quad (C-8a)$$

where T_c is the critical temperature and T_b is the boiling point of the compound of interest, both in °C. ΔH_{VB} (cal/mol) is the molar heat of vaporization at the normal boiling point and is estimated using the method of Haggenmacher (Lyman et al. 1990, Section 13-5):

$$\Delta H_{VB} = \frac{2.303BR(T_b + 273.2)^2(z_g - z_l)}{(T_b + C)^2} \quad (C-9)$$

where:

$$z_g - z_l = \sqrt{1 - \frac{(1/P_c)}{[(T_b + 273.2)/(T_c + 273.2)]^3}} \quad (C-10)$$

where T_c is the critical temperature in °C, P_c is the critical pressure in atm, B and C are Antoine's constants; B is in °C or K and C is in °C. Antoine's constants have been calculated for many compounds, especially hydrocarbons, and are tabulated in the literature (e.g. (Reid et al., 1977)). In some tabulations, the conversion factor to natural log (2.303) is included in the value of B. To check, if the value for methane is 405.42 (°C or K) use the values for B directly. If it is about 930 (°C or K), divide all values for B by 2.303. Also, if Antoine's constants are presented in the literature in K, B *should not be changed*, and C should be converted to °C by *adding* 273.2. Note that this is not the usual way to convert from K to °C, but is necessary to maintain the constancy of the term $B/(t+C)$ in Antoine's relationship since temperature, t , is assumed to be in °C.

In the code, if T_c and P_c are unavailable, but B and C are available, $(z_g - z_l)$ is approximated as one (Lyman et al., 1990, Table 14-6). If only T_c is unavailable, T_c (°C) is estimated as $(1.5T_b - 136.6)$ (Lyman et al., 1990, p. 14-13). If T_c , P_c , B, and C are all unavailable, Trouton's rule is used to estimate ΔH_{VB} (cal/mole) (Lyman et al. (1990):

$$\Delta H_{VB} = 21 \frac{\text{cal}}{\text{mole K}} * (T_b + 273.2) \quad (C-11)$$

Table C-1: Summary of input parameters

Symbol	Units	Definition
$K_H(T_{K_H})$...	dimensionless Henry's Law coefficient at T_{K_H}
T_{K_H}	°C	temperature at which K_H was evaluated
T_b	°C	boiling point
T_c	°C	critical temperature
P_c	atm	critical pressure
B	°C or K	Antoine constant
C	°C	Antoine constant
V'_B	cm ³ /mole	LeBas molar volume
MW	g/mole	molecular weight

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APPENDIX D:
SOILRISK: DETAILS OF THE DUST GENERATION MODULE

The dust generation model is based on the procedure developed by Cowherd et al. (1985) was adapted for implementation in a computer code and is presented in detail here. The input parameters required for the module can be categorized as those describing the surface of the site, the climate at the site, and the activities or exposure conditions occurring at the site. They are summarized in Table D-1. Where applicable, sources of information regarding the appropriate values for the input parameters are referenced or the information is provided.

Table D-1: Summary of input parameters to the dust generation module

Symbol	Units	Definition
(a) Properties of the surface of the site		
asdm	mm	mode of the aggregate size distribution
Lc	...	ratio of the silhouette area of roughness elements to total base area
v	...	fraction of surface covered with vegetation
z0	cm	roughness height
s	%	silt content of site surface
Area	m ²	surface area of the contaminated site
(b) Climatological parameters		
U ⁺	m/s	fastest mile of wind (m/s)
PE	...	Thornthwaite Precipitation Evaporation Index
\bar{u}	m/s	annual average surface wind speed
p	d/yr	mean no. of days with at least 0.01 in precipitation
(d) Exposure parameters		
fd	1/mo.	frequency of disturbances per month
tr	km	distance of travel over contaminated site
T	veh/d	average number of vehicles per day
Sp	km/hr	mean vehicle speed
Wt	Mg	mean vehicle weight
wh	...	mean number of wheels per vehicle

STEP 1: CALCULATE U_{*t}

Calculate the threshold friction velocity, U_{*t} , the threshold wind speed for the onset of wind erosion in m/s.

$$U_{*t} = cf \cdot 0.650 \cdot (asd_m)^{0.425} \quad (D-1)$$

where:

$$cf = \begin{cases} 0 & Lc < 2.0 \times 10^{-4} \\ 1.05 + 50.18 \cdot Lc - 647.89 \cdot Lc^2 + 6863.50 \cdot Lc^3 & 2.0 \times 10^{-4} \leq Lc \leq 10^{-1} \end{cases} \quad (D-2)$$

where asd_m is the mode of the aggregate size distribution in mm and Lc is the ratio of the silhouette area of roughness elements too large to be included in sieving to total base area.

This is measured by inspection of a representative one meter square transect of the site surface. Cowherd et al. (1985) provides examples. Lc can range from zero to 0.01.

Equations D-1 and D-2 were derived from Figures 3-4 and 3-5 in Cowherd et al. (1985).

STEP 2: CALCULATE U_t

U_t is the threshold wind velocity in m/s at a height of 7.0 m.

$$U_t = \frac{1}{0.4} \ln \left(\frac{700}{z_0} \right) U_{*t} \quad (D-3)$$

where z_0 is the roughness height in m. Values for z_0 for various surface conditions are provided in Figure D-1.

STEP 3: CALCULATE E10W:

E10w is defined as the annual average emission rate of particulate matter less than 10 μm in diameter (PM10) per unit area of the contaminated surface due to wind erosion. Units are $\text{g}/\text{m}^2\text{-hr}$.

If $U_{*t} > 0.75 \text{ m/s}$

In this case, the site is considered to have limited erosion potential and the following equation is used to calculate E10w. It was derived by combining equations 4-1 to 4-3 in Cowherd et al. (1985).

$$E10w = \begin{cases} \frac{5.56(U^+ - U_t)(1-v)fd}{PE/50^2} \cdot \frac{1}{10^3} & U^+ > U_t \\ 0 & U^+ \leq U_t \end{cases} \quad (D-4)$$

where U^+ is the fastest mile of wind in m/s, v is the fraction of the contaminated surface covered by vegetation (0 for bare soil), fd is the frequency of disturbances per month, PE

is Thornthwaite's Precipitation Evaporation Index used here as a measure of the average surface soil moisture content. In the definition of f_d , a disturbance is defined as an action which results in exposure of fresh surface material. Data for U^+ and PE for locations throughout the US can be found in climatic atlases (e.g., U.S. Department of Commerce, 1968) and Figure D-2 respectively. Cowherd et al. (1985) advise that in the worst case, f_d should be assumed to be 30 per month.

If $U_{*t} \leq 0.75$ m/s

If $U_{*t} \leq 0.75$ m/s, the site is considered to have unlimited erosion potential and E_{10w} is calculated using:

$$E_{10w} = 0.036(1 - \nu) \left(\frac{\bar{u}}{U_t} \right)^3 g(x) \quad (D-5)$$

where:

$$x = 0.886 \frac{U_t}{\bar{u}}$$

$$g(x) = \begin{cases} 1.91 & 0 \leq x < 0.5 \\ 2.2 - 0.6x & 0.5 \leq x \leq 1.0 \\ 2.9 - 1.3x & 1.0 \leq x \leq 2.0 \\ 0.18(8x^3 + 12x)\exp(-x^2) & x > 2.0 \end{cases} \quad (D-6)$$

and \bar{u} is the mean annual wind speed in m/s. Data for \bar{u} for locations throughout the US can be found in climatic atlases (e.g., U.S. Department of Commerce, 1968).

STEP 4: CALCULATE E_{10vt}

E_{10vt} is defined as the annual average PM₁₀ emission rate caused due to vehicular traffic on unpaved roads. Units are gram per vehicle-km of travel, g/vkt. Equation 4-7 (p.37) in Cowherd et al. (1985) is used:

$$E_{10vt} = 850 \left(\frac{s}{10} \right) \left(\frac{Sp}{24} \right)^{0.8} \left(\frac{Wt}{7} \right)^{0.3} \left(\frac{wh}{60} \right)^{1.2} \left(\frac{365 - p}{365} \right) \quad (D-7)$$

where s is the percent silt content of the road material, Sp is the mean vehicle speed in km/hr, Wt is the mean vehicle weight (Mg) and wh is the mean number of wheels per

vehicle, and p is the mean number of days with at least 0.254 mm (0.01 in) of precipitation per year (day/yr). Data for p for locations throughout the US can be found in climatic atlases (e.g., U.S. Department of Commerce, 1968). Default values for s , Sp , Wt , and wh are reproduced Table D-2.

Table D-2: Default Values and Ranges for Inputs to Eq. D-7 (Cowherd et al., 1985)

Site	$s(\%)$	$Sp(\text{km/hr})$	$Wt(\text{Mg})$	wh
Rural/Resid	15(5-68)	48(40-64)	2	4
Industrial	8(2-29)	24(8-32)	3	4
			15	6
			26	10

STEP 5: CALCULATE R10T

R10T is the total annual average emission rate of PM10 from the site in g/s.

$$R10T = \frac{E10W \cdot \text{area}}{3600} + \frac{E10vt \cdot tr \cdot T}{86400} \quad (\text{D-8})$$

where area is the surface area in m^2 , tr is the distance of travel over the contaminated site in km, T is the average number of vehicles traveling over the contaminated surface per day (vehicles/day).

R10T in g/s is input to the onsite air dilution model to determine the average PM10 concentration above the site which then used in the dust intake calculation.

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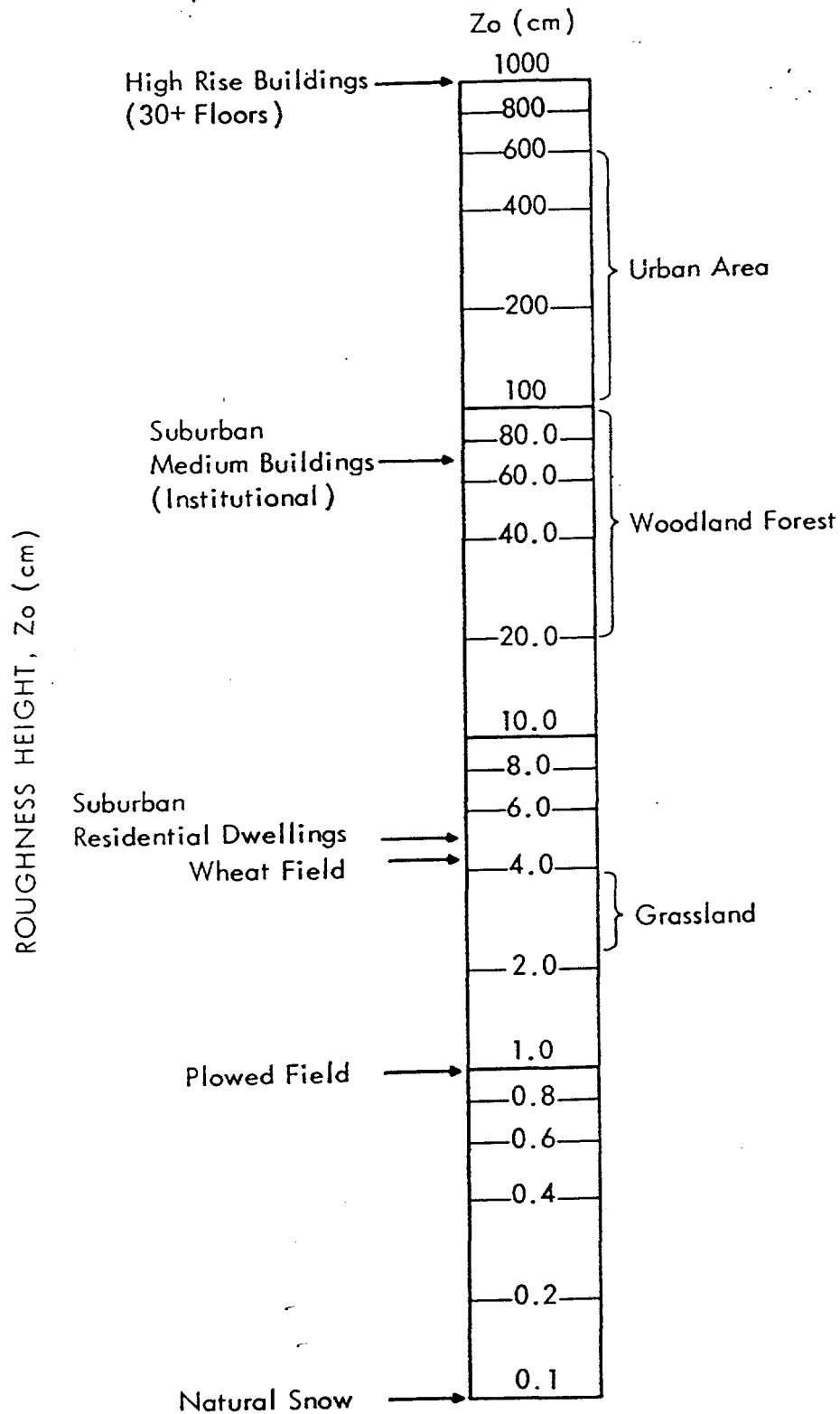


Figure D-1: Roughness Heights, Z_0 , for various surfaces.
(from Cowherd et al., 1985)

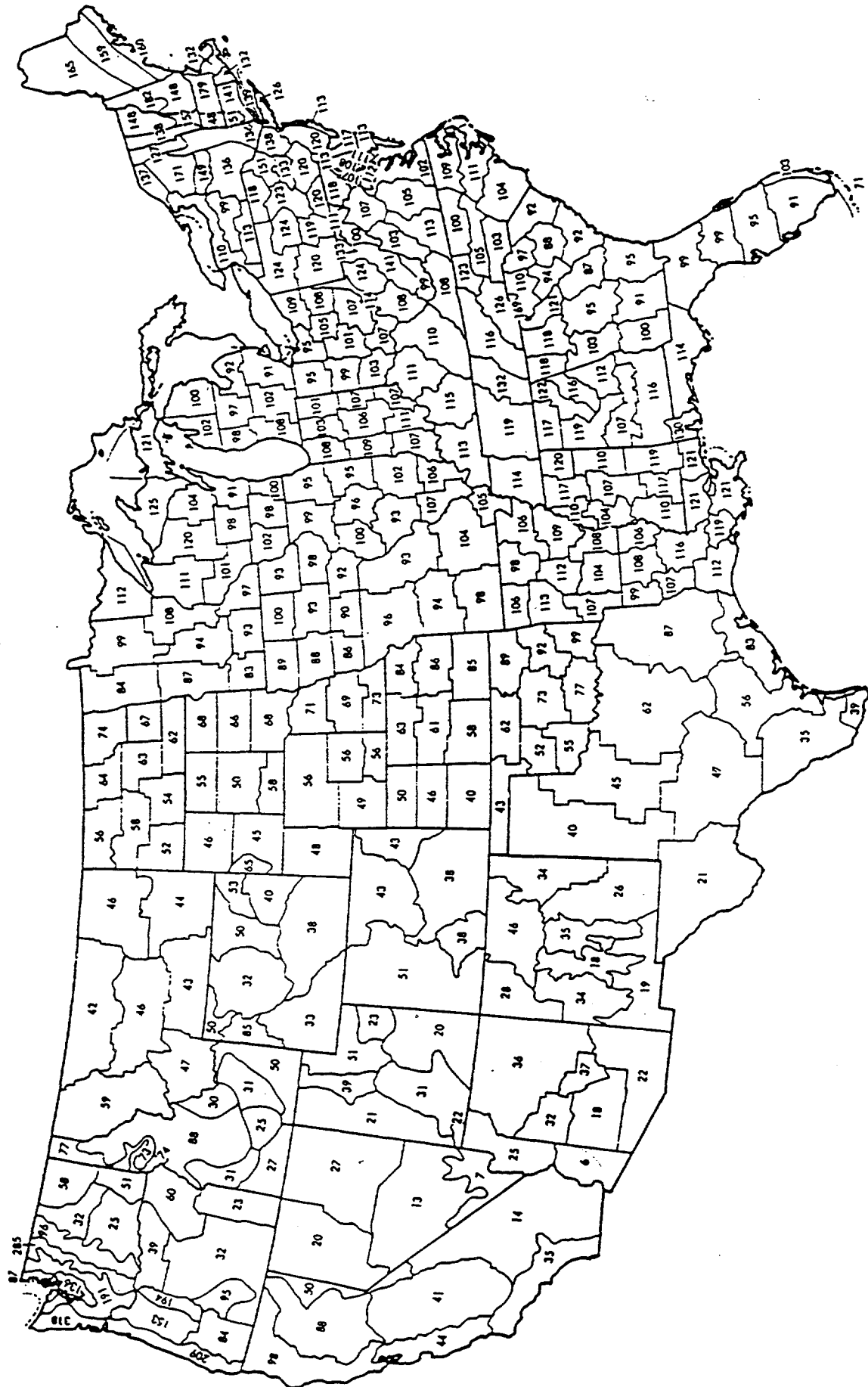


Figure D-2: Map of Thornthwaite's PE Index for State Climatic Divisions (from Cowherd et al., 1985)

APPENDIX E:
DEFINITION OF SOIL USED IN SPECIFYING SOIL
REMEDICATION GOALS

INTRODUCTION

Soil remediation goals are *in-situ* concentration levels. Since soil in the ground consists of multiple phases (solid, liquid, and gas), each of which can contain contaminants, it is critical that soil remediation goals be consistent with soil sampling and analysis methods and vice versa. Currently, this is not the case and confusion abounds as to the technical meaning of a soil concentration. Does it include the solids, the pore liquids, and the pore gas? While the total contamination in the solid phase, the gas phase, the aqueous phase, and the free organic liquid phase can be measured, it is not at all clear that this should be the basis for soil quality criteria. Obviously, standardized soil sampling and analysis techniques that are consistent with an unambiguous definition of soil are required.

U.S. EPA GUIDANCE

A review of the literature reveals that the exact definition of soil depends on one's perspective. To the traditional soil scientist, it is a medium for plant growth which includes four components: mineral matter, organic matter, water, and air. To the geo-technical engineer, it is foundation material for engineered structures, roads, etc.. To the hydrogeologist, it is a porous medium allowing subsurface flow.

EPA guidance on soil sampling provides the following definition of soil:

... the surface and subsurface mass of unconsolidated mantle of weathered rock and loose material lying above solid rock. The soil component can be defined as all mineral and naturally occurring organic material less than 2 mm in size. This is the size normally used to distinguish between soil (e.g. sands, silts, and clays) and gravels. (Barth et al., 1989, Ch 2, p. 9)

Note that this definition refers exclusively to the solid phase components and omits the liquid and gas phase components of soil.

EPA guidance on the sampling of waste solids, which includes contaminated soil, adds that a sample should include "any entrapped gases or fluids" (U.S. EPA, 1984). This definition plainly contradicts that given above. Moreover, soil sample analysis methods are often inconsistent with one or both of these definitions because they call for partial removal of liquids (e.g. filtering, but not drying required) or they allow volatilization losses, which are particularly critical when measuring volatile organic compounds. An example of the latter problem is embodied in the current Method 8240, a general analytical methodology for VOCs in solid samples specified by the U.S.EPA, which prescribes homogenizing samples in a pan prior to taking an aliquot (U.S. EPA, 1986). This procedure obviously allows volatilization losses. Some studies have shown that there is considerable variation on sample results when different sample collection and handling procedures are used (Siegrist and Jensen, 1990).

SOIL DEFINITIONS IN TCE SITE DOCUMENTATION

Clear technical definitions for soil were not found in the site documentation of the TCE contaminated sites reviewed (Appendix F) either. The definition of a soil contaminant concentration used in cases where the Summers model (Summers et al., 1980), the MULTIMED model (Salhotra et al., 1990) , and equilibrium partitioning were used to establish the soil goal is *implicitly* the mass of contaminant adsorbed onto the solid phase of the soil per unit dry mass of soil. Site documentation was also reviewed to determine if sample collection and analytical methods specified for measuring contaminant concentrations in soil are consistent with this implied definition. According to discussions with RPMs analytical methods are specified in the design phase. Design phase documents are not available in the Administrative Record and were not obtained.

In the review of TCE contaminated sites, it was also noted that there is also lack of clarity in whether the soil remediation goal established is applicable in the unsaturated zone, the

saturated zone, or both. At all of the sites, it is clear that the soil goal applies to the unsaturated zone. However, it is unclear whether the soil goal is to be applied to the saturated zone as well. In most cases, separate remediation strategies have been developed for the unsaturated zone, commonly in-situ vapor extraction (ISVE), and contaminated groundwater, universally groundwater pump and treat schemes. (Site remediation strategies at the site reviewed are summarized in Appendix F, Table F-7). It is commonly stated that ISVE will continue until the soil remediation goals are met (in the unsaturated zone) and that the pump and treat strategy will continue until the groundwater goals are met, with no mention of the soil goals being attained in the saturated zone. At a few sites there is explicit remediation of the saturated soils via drawdown and in situ vacuum extraction (ISVE) or by recharging treated groundwater through the contaminated zone. In these cases, it is implied that the remediation will continue until the soil cleanup goals are attained in the saturated as well as the unsaturated zone.

In addition to reviewing site documentation for an exact definition of soil, six site RPMs and a hydrogeologist in one of the regional offices were asked about the definition of soil used in establishing the soil remediation goals at their sites. Five out of the six were not sure what definition of soil was used. One said that it is the unconsolidated material at the site, drained and excluding rocks and debris. The hydrogeologist questioned said that it is the unconsolidated material above the water table.

SUMMARY

Clear USEPA guidance on the definition of soil is clearly lacking. The results presented in this section illustrate both the ramifications of a lack of clear guidance as well as the need for it.

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APPENDIX F:
REVIEW OF TCE CONTAMINATED SITES

A review of sites with TCE contamination in soil was performed in order to identify a generalized site profile and to document the current methodologies being used to establish soil remediation goals for TCE and the range of goals being set.

TCE has been chosen because it is one of the most common contaminants found at CERCLA sites (Grisham, 1986; Siegrist, 1992) as well as at U.S. Department of Energy sites (Riley et al., 1992), it is classified as a probable human carcinogen by the U.S. EPA due to significant increases in the incidence of liver tumors in mice upon exposure to it (U.S. EPA, 1988; U.S. EPA, 1991), and it is representative in its fate and transport properties of other chlorinated aliphatics and volatile organic compounds.

Existing CERCLA site databases and reviews were consulted to identify those sites where soil contamination with TCE has been detected and where a soil remediation goal for TCE has been or will be established. It was not the objective to provide an exhaustive review of sites fitting this description, but rather to get enough information on a range of sites to accomplish the stated goals.

IDENTIFICATION/DOCUMENTATION OF SITES

Most sites were identified by searching the Records of Decision (RODs) Database maintained by the U.S. EPA and HAZDAT, a database developed by the University of Tennessee and available through the Oak Ridge National Laboratory (ORNL). A few sites were identified through a past review of site cleanup levels (Baes and Marland, 1989) and by speaking with EPA Remedial Project Managers. The search of the RODs database was limited to U.S. EPA Regions 1 (CT, ME, NH, RI, VT), 2 (NJ, NY, Puerto Rico, Virgin Islands), 3 (DE, MD, PA, VA, WV), and 5 (IL, IN, MI, MN, OH, WI) to facilitate access to documentation. Detailed information for many of the sites identified in the database searches was obtained by visits and Freedom of Information Act (FOIA) requests to the

U.S. EPA Regional Offices. These offices maintain Administrative Records for the Superfund sites in their respective regions for which RODS have been issued. The Administrative Record for a site contains all documentation leading up to a ROD.

A total of 21 sites was identified. The sites identified and the documents reviewed for each site are presented in Table F-1. For each site identified, information was obtained from review of RODs, supporting documentation such as the EPA Remedial Investigation/Feasibility Studies, and from phone conversations with the Remedial Project Managers. It should be noted that different amounts of site information were obtained for each site. This is due to the fact that in some cases the site information was readily available from a visit Administrative Record or from cooperative RPMs. In other cases, complete site information was not readily available, but the site was kept on the list of sites of interest because at least there was information on some aspect of the site that was useful for this review. For example, there were cases where information was available on the soil clean up goal established for the site from the ROD Abstract available from the RODS Database, but no information was obtained on the details of the site hydrogeology.

SUMMARY OF SITE CHARACTERISTICS

The range of site characteristics at the sites identified for this study are reported and discussed below.

Subsurface profile

Table F-2 provides a summary of the subsurface profiles at each of the sites where such information about the site was obtained. A wide variety of subsurface profiles are apparent. The hydrogeological parameters describing the uppermost unconfined aquifer at each of the sites are also tabulated.

Despite the wide range of properties and profiles, some generalizations are possible. With one exception, at the sites for which information is reported, the contaminated area sits on top of an unconfined, unconsolidated aquifer which in turn sits on either a confining layer, a rock aquifer, or relatively impermeable bedrock. The exception to this is the Acme Solvent Site where the uppermost aquifer below the contaminated area occurs in fractured bedrock. The sites which have unconsolidated, unconfined aquifers have a fairly shallow depth to the water table. The average is approximately 10 feet. The average thickness of the unconsolidated aquifer is about 30 feet. The hydraulic gradient is fairly low, with an average of roughly 1×10^{-2} . Nine out of the 15 sites for which information about the subsurface profile was available have aquifer material consisting of silty sands, sands, or sand and gravel. The hydraulic conductivity (K) ranges over four orders of magnitude, from 0.028 to 570 ft/day, with an average of 95 ft/day. (In m/s, the range is 2×10^{-3} m/s to 1×10^{-7} m/s, which corresponds to the lower bound for sands and gravels down to the lower bound for silty sands in Freeze and Cherry(1979),p. 29). The average porosity reported is 0.3, the average weight fraction organic carbon content of the soil is 0.02 (excluding Greenwood Chemical which reports a very high Foc of 0.1). It should also be noted that at the 15 sites where information was available on the use of groundwater, the groundwater at or near the site is being used for drinking water.

Surface hydrology

Table F-3 provides a very brief summary of the major features of the surface water hydrology at each of the sites. The effect of the surface hydrology on the subsurface hydrology is also noted. It is common to have a wetland (5 sites), creek (5 sites), or river (5 sites) on or near the site. The only surface hydrology features mentioned at 2 sites are drainage ditches. It was not possible to generalize about the type of surface water present, its proximity to the site, and its relationship to the subsurface hydrology.

Contaminant distribution

Table F-4 gives an overview of the distribution of TCE detected in soil, groundwater, and surface water, and air. At all sites reviewed, TCE was detected in soil. This is obvious since this was one of the criteria used to choose the sites. However, most sites show only subsurface soil contamination with TCE. (The definition used for subsurface in the reports reviewed varies from greater than 6 inches to greater than 2 feet below grade.) If surface soil contamination was detected, it was present in much lower concentrations than the subsurface soil contamination. Additionally, in all cases where TCE contamination was detected in soil, it was also detected in groundwater. This is true regardless of the cause of contamination: surface spills or leaks, dumping in excavated area, leaking underground storage tanks, or the use of a leach field. With regard to surface water contamination, in most cases, either no information was available on the sampling or detection of TCE in surface water, or surface water was not sampled for TCE contamination. The air was reported to have been sampled at only three sites. At all three of these sites, no TCE in air was detected. It should also be noted that at all sites, multiple contaminants have been detected in soil and groundwater.

The possible presence of pure phase TCE in a separate non-aqueous phase is explicitly mentioned in the documentation reviewed for only three of the sites. At the Verona Wellfield, a light non-aqueous phase liquid (LNAPL) as much as 4 ft thick has been detected. Although TCE has a specific gravity of 1.46, it has been detected in the floating LNAPL in a mixture with other VOCs whose specific gravities are less than 1.0. At Tyson's Dump, there is discussion of the possibility of dense non-aqueous phase liquid (DNAPL) migration to bedrock, but no pure phase has been detected. At the Byron Barrel and Drum site, there is acknowledgment of the possible presence of a DNAPL layer and a discussion of the evidence against it. The evidence listed is: 1) the maximum concentration of TCE detected in the groundwater is 3,300 ppb which is only 0.3% of the aqueous

solubility of TCE, and 2) greater TCE concentrations have been detected in shallow rather than deep monitoring wells. At another site, Groveland Wells 1 and 2, there is acknowledgment of the possible presence of contamination trapped in the soils above a clay layer. There is no explicit discussion of the presence of a DNAPL, however.

To generalize, review of the sites examined in this study indicates that where TCE contamination in soil exists, TCE contamination of groundwater also exists regardless of the initial cause of contamination. No generalizations about the migration of TCE to air and surface water can be made since there are very little data available on this. It is also not possible to make generalizations about the presence of TCE as a DNAPL, since this possibility is not addressed at most sites.

Contaminant fate and transport processes

The major fate and transport processes considered in developing a remedial strategy for soil at all the sites where relevant documentation was obtained were adsorption of TCE onto soil, infiltration by precipitation, leaching of adsorbed contamination from soil, mixing with groundwater, and advection and dispersion of dissolved solute in the saturated zone.

GENERALIZED SITE PROFILE

A simple generalized site profile of a TCE contaminated site can be developed from the observations listed above and in Tables F-2-F-4 and site documentation. The typical site is underlain by an unconfined, unconsolidated aquifer consisting of silty sand, sand, or sand and gravel with porosity of about 0.3, and an F_{oc} of about 0.02. The water table occurs at a depth of roughly 10 feet and the thickness of the aquifer is roughly 30 feet. The hydraulic gradient is fairly low, on the order of 10^{-2} . The groundwater at or near the site serves as a potable water supply. TCE contamination has resulted from surface spills, leaks and dumping into excavated areas. The area of contamination is highly variable, but

averages $5.3E4 \text{ ft}^2$. TCE contamination occurs in both the soil and the groundwater. The generalized site profile is summarized in Table F-5.

Table F-5: Generalized site profile	
Descriptor	
unsaturated zone media	sandy
saturated zone media	sandy
n	0.3
Foc	0.02
depth to water table (ft)	10
height of aquifer (ft)	30
i	10^{-2}
K (ft/day)	95
Area (ft^2)	$5.3E4$

SOIL REMEDIATION GOALS

Summary of goals and methods used

Table F-6 summarizes the established clean up goals, the basis for them, and the models used. Soil cleanup goals have been established for 18 of the 21 sites. The cleanup goals for the remaining three sites are to be determined in the design phase of the remedial action. The reports on these were not yet available. The cleanup levels established range from 5 to 2000 ppb, a notably wide range.

At four out of the 21 sites, the soil goal was established based on state guidelines (in Michigan and New Jersey). At one site, the soil goal was established based on a consent agreement between the potentially responsible party and USEPA. At the remaining 16 sites, achieving a specified contaminant concentration in groundwater was cited as the basis for the soil goal established or to be determined. However, at such sites, there are differences in:

- 1) specified contaminant concentration in groundwater.

It is the MCL at 10 sites, the groundwater concentration established by the state for the two sites in Wisconsin, a contaminant concentration to achieve a specified risk

goal due to the ingestion of groundwater at another two sites, and a contaminant concentration in groundwater established by consent agreement between the responsible parties and the EPA at one site.

2) specification of where the groundwater goal is to be attained.

In most cases (10 out of the 16 sites) the groundwater goal is to be achieved in the uppermost aquifer directly below the site. In these cases, the fate and transport processes considered are infiltration by precipitation, leaching of adsorbed contaminant from the soil solid phase, and mixing with groundwater. At one site, American Thermostat, a contaminant concentration in groundwater at a distance of 180 feet from the well was cited as the basis. In this case, the fate and transport processes of adsorption, and advection and dispersion of dissolved solute in the saturated zone were considered in addition to those listed above. In two other cases, Bendix Flight Systems and Pristine, the groundwater goal was specified to be achieved in aquifers below the uppermost unconfined aquifer

3) fate and transport models used to estimate the contaminant concentration in soil that will achieve the specified groundwater goal at the specified distance from the contaminated area

Nine out of the 13 sites that use some kind of fate and transport model use the Summers model, where the contaminant concentration in the soil-water is determined from equilibrium partitioning and a simple dilution model is applied to determine the groundwater contaminant concentration below the site (Summers et al., 1980). The MULTIMED model (Salhotra et al., 1990) (See Appendix A for a brief description) was used at one site, and equilibrium partitioning was the cited approach at the remaining 2 sites. At Bendix flight systems, no formal model was presented. Rather, 100-fold dilution was assumed to occur between the shallow glacial till aquifer and the bedrock aquifer at the site. No justification for this

assumed relationship could be found in site documentation nor through a FOIA request.

As these results indicate, a risk assessment where the soil goal is calculated to achieve a particular level of risk was not performed at most of the study sites. Rather, a previously established groundwater concentration goal was used as the basis and an environmental fate and transport model was applied using site specific parameters to estimate the contaminant concentration in soil that would achieve the groundwater goal. Where a risk assessment was performed to determine a contaminant concentration in soil to meet a risk goal, the risk due to only one exposure route, groundwater ingestion, was considered. In some cases, a soil clean up level to meet a 10^{-6} risk level due to soil ingestion only was calculated in addition to the groundwater-based soil cleanup level. In all cases where this was done, the latter was an order of magnitude or more lower than the former. That is, the groundwater exposure route was identified as the critical one.

In most cases there is poor documentation of the method used to establish the clean up goal. In a few cases, even where a simple model like the Summers model is used, the soil cleanup goal could not be reproduced due to poor documentation (e.g., Main Street Wellfield).

Even though the Summers model was the most common model used to relate contaminant concentrations in soil to concentrations in groundwater for the sites evaluated, there appears to be very little consistency in how it is applied. There are differences in:

- the choice of the aquifer in which the groundwater goal should be attained.

At the Pristine site, an unconsolidated unconfined aquifer overlies a lower confined aquifer. The lower aquifer was chosen as the aquifer of concern, and the Summers

model was applied as if the unconfined aquifer above it didn't exist. In most other cases, the Summers model was applied to the uppermost unconfined aquifer.

- the choice of the mixing zone.

At one site the depth of the screened zone in the monitoring wells was used (Byron), at another the screened depth of the nearest drinking water well was used (Pristine), at others the full depth of the unconfined aquifer was used.

- how site properties are averaged for use in the calculation.

At some sites, all the measurements for site properties such as K (e.g., Main Street Wellfield) were averaged while others used an extreme value (e.g. Byron and Pristine used the maximum measured K).

- specification of the area of contamination.

At some sites (e.g. Pristine) the contaminated area was assumed to be the whole site whereas at others a contaminated area was specified based on preliminary measurements such as a soil gas survey (e.g., Byron). At one site, Enviro-Chem, a contaminated area of 1m by 0.63m was assumed with no justification. In the cases where only a portion of the site is considered, the goal was meant to apply to the whole site.

- assumptions about the background contaminant concentration in the aquifer.

At Zanesville Wellfield, it was assumed to be 5 µg/l; all others assume 0 µg/l.

It was also noted in this review that there is no consistent definition of soil and of the soil contaminant concentration to be used as a remediation goal. This issue is discussed more fully in Appendix E.

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Table F-1: List of sites and information reviewed.

Site Name	City	St	EPA Reg	ROD Date	Site Information obtained from: (2)					Other
					OU (1)	Abstract	ROD	ROD	RI/FS	Phone conversation w/ RPM (name, date of contact)
Main Street Wellfield	Elkhart	IN	5	3/29/91	2	X	X	X	X	Cindy Nolan, 8/11/92
Zanesville Wellfield	Zanesville	OH	5	9/30/91	-	X	X	X	X	Dave Wilson, 9/3/92
Verona Wellfield	Battlecreek	MI	5	6/28/91	2	X	X	X	X	Margaret Guerriero, 8/7/92
Enviro-Chem	Zionsville	IN	5	6/7/91	-	X	X	X	X	Karen Vendl, 8/7/92
Acme Solvent Reclaiming	Winnebago	IL	5	12/31/90	2	X	X	X	-	(3)
Springfield Twp Dump	Springfield Twp	MI	5	9/29/91	-	X	X	X	-	-
Fisher-Calo Chem	Kingsbury	IN	5	8/7/90	-	X	X	X	-	-
Wayne Waste Oil	Columbia City	IN	5	3/30/90	-	X	X	X	-	Tinka Hyde, 8/11/92
Pristine, Inc	Reading	OH	5	3/30/90	-	X	X	X	X	-
Oconomowoc Electroplating, Inc	Ashippun	WI	5	9/20/90	2	X	X	X	-	Thomas Williams, 9/3/92
Wausau Groundwater Contamination	Wausau	WI	5	9/29/89	1	X	X	X	-	Margaret Guerriero, 10/5/92
Metaltec-Aerosystem	Franklin Boro	NJ	2	6/30/86	-	X	-	-	-	(4)
Greenwood Chemical Site	Newtown	VA	3	12/29/89	1	X	X	X	-	Phil Rotstein, 8/2/92
Tyson's Dump	Upper Merion	PA	3	3/31/88	-	X	X	X	X	Eugene Dennis, 4/7/92
Byron Barrel and Drum	Byron	NY	2	9/29/89	-	X	X	X	X	Eddie Gonzalez, 9/4/92
Fulton Terminals	Fulton	NY	2	9/29/89	-	X	-	-	-	Christos Tsiamos, 7/16/92
American Thermostat	Green County	NY	2	6/29/90	2	X	-	-	-	Christos Tsiamos, 10/8/92
Groveland Wells 1&2	Groveland	MA	1	9/30/88	1	X	X	-	-	(6)
Waldick Aerospace Devices	Wall Twp	NJ	2	9/29/87	1	X	-	-	-	John Prince, 7/16/92
Caldwell Trucking	Fairfield	NJ	2	9/25/86	1	X	-	-	-	Ed Finnerty, 7/31/92
Bendix Flight System	South Montrose	PA	3	9/30/88	-	X	X	X	-	Humane Zia, 3/27/92

Notes:

(1) OU= operable unit

(2) ROD Abstract in the RODS Database, RI/FS=Remedial Investigation/ Feasibility Study, RPM= USEPA Remedial Project Manager.

(3) Harding Lawson Associates. (1990). *Remedial Action Alternatives Evaluation Final Report Acme Solvents Site, Winnebago County, Illinois*, Vol.II of II. . Prepared for Acme Solvents Steering Committee, Chicago, Illinois. Denver, Colorado. Prepared by Harding Lawson Associates, Denver, Colorado.(4) Baes, C. F., & Marland, G. (1989). *Evaluation of cleanup levels for remedial action at CERCLA sites based on a review of EPA Record of Decision* (Environmental Sciences Division Publication No. 3104). Oak Ridge National Laboratory.(5) Clement Associates Inc. (1989). *Cleanup Goals for the Greenwood Chemical Site Albemarle County, Virginia*. Prepared for EBASCO Services, Inc., Arlington, Virginia. Prepared by Clement Associates Inc., Fairfax, Virginia.

- (6) HAZDAT Database maintained by Oak Ridge National Laboratory, Oak Ridge, Tennessee.
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Table F-2: Site subsurface profiles and hydrogeologic data.

Name	Subsurface Profile (1, 2)	Hydrogeologic properties of uppermost unconfined aquifer (4)					
		Depth to Aquifer wt (ft)	Porosity ht (ft)	Foc (5)	K (ft/day)	i (-)	Area (ft ²)
Main Street Wellfield	50' sand and gravel(wt)/ 100' impermeable till (silty clay, clay)/ shale	8 to 15	42 to 58	0.25	0.004	85 to 396	3.00E-3 to 2.70E+04
Zanesville Wellfield	5-10' clayey alluvium/ 5-20' sand and gravel/20-40' sand (wt)/15-30' sand and gravel/ shale	10 to 30	45	0.3	0.01	384 to 571	2.00E-2
Verona Wellfield	10-50 fine to med sand with gravel and silt(wt)/100-120 sandstone aquifer / shale. (Small downward gradient to sandstone aquifer (K=28 - 595 ft/day, i=2.2e-3)).	8 to 28	0 to 40	0.25 to 0.40	0.0014	70.9	2.70E-03
Enviro-Chem	-	-	-	-	-	0.028	2.00E-02
Acme Solvent Reclaiming	0-6' unconsolidated deposits/ 220' dolomite (wt)(flow in fractures)/ 40' semi-confining layer (shale and quartz sandstone)/ 320' sandstone aquifer (intergranular flow)	20	200	-	0.03	2.27	4.00E-03
Springfield Twp Dump	shallow and deep aquifer	-	-	-	-	-	-
Fisher-Calo Chem	-	-	-	-	-	-	-
Wayne Waste Oil	-	-	-	-	-	-	-
Pristine, Inc	0-10' fill/ 0-46' upper lake sediment is upper aquifer (wt) consists of three perched water systems within three outwash lenses all interconnected/ 10-45' glacial till/ 15' lower lake sediment/ lower outwash deposit or lower aquifer.	8 to 12	0 to 46	0.3	0.005	139	2.45E-03
Oconomowoc	30-60' unconsolidated deposits (wt)/ 0-30' upper dolomite 5 aquifer/ 40' shale/ lower dolomite aquifer	25 to 55	-	-	-	-	9.60E-04
Wausau Groundwater	glacial outwash and alluvial sand(wt)/ bedrock valley	-	0 to 60	-	-	0.48 to 230	-
Metaltec-Aerosystem	-	-	-	-	-	-	-
Greenwood Chemical Site	-	-	25	-	0.1	0.86	3.00E-02
Tyson's Dump	Below lagoon: <2'slag and sand fill/ bedrock aquifer. Below lower area toward river: <1' topsoil/~ 6' clayey sand to sandy silt/~5' fine to med sl silty sand some gravel/ bedrock aquifer. (Bedrock highly fractured)	1.5 to 16.7	-	0.35	1.1	5.35E-02	4.60E+04
Byron Barrel and Drum	3-31' org soil with silty sand (K=0.64 to 81 ft/day) (wt) / 50' glacial till (K=5.5e-3 to 1.1e-2 ft/day)	3 to 11	20	0.2 to 0.3	0.0089	73	1.80E-03

Table F-2: Site subsurface profiles and hydrogeologic data. (cont'd)

Name	Subsurface Profile (1, 2)	Hydrogeologic properties of uppermost unconfined aquifer (4)					
		Depth to Aquifer wt (ft)	Aquifer ht (ft)	Porosity (5)	Foc (5)	K(ft/day) i(-)	Area(ft ²)
Fulton Terminals	4-12' artificial fill (sand and gravel)/ 0-25' silt and clay/ 25-58' sand and gravel/ bedrock.	-	-	-	0.06	32	5.00E-03 7.85E+03
American Thermostat	unconsolidated glacial deposits(wt)/ bedrock aquifer	4	40	0.3	0.06	1.4	1.80E-02 3.00E+04
Groveland Wells 1&2	2-4' med to fine sand and gravel/ 4-8' ablation till/ 2-10' clay lense (under portion of site)/ 8-10' compacted sand and gravel outwash/ 2-4' basal or lodgement till/bedrock (total: 32-50' to bedrock)	25 to 30	-	-	-	-	2.50E+04
Waldick Aerospace Devices	Two aquifers separated by a 'somewhat' permeable clay layer which is 35-30' below grade.	-	-	-	-	-	-
Caldwell Trucking	-	-	-	-	-	-	-
Bendix Flight System	14-70' glacial till (wt)(poorly sorted, varying from from dense sand and silt to hard silt and gravel till with varying amounts of clay and a little sand)/ fractured bedrock aquifer.	2 to 10'	-	-	-	-	-

Notes:

- (1) wt=water table
- (2) - = no information given in documentation obtained.
- (3) Hydrogeologic properties given are for the lower aquifer.
- (4) Foc=fraction organic carbon, K=hydraulic conductivity, i=hydraulic gradient. Average or range given.
- (5) Note that half the foc measurements are assumed values (Main,Acme, Pristine, Greenwood), all porosity values are assumed.

Table F-3: Summary of site subsurface hydrology.

Name	Surface water description	Effect on subsurface hydrology (1)
Main Street Wellfield	Bounded by river to South, tributary creek through site.	GW discharge to creek or river.
Zanesville Wellfield	River runs thru site.	GW discharges to river. Pumping in wellfield reverses this.
Verona Wellfield	River runs thru site.	River recharges sand and gravel aquifer in some areas. In others GW flow is to river. Affected by zone of influence of wellfield.
Enviro-Chem	Runoff to ditch which flows to Creek, then goes 10 miles to a drinking water reservoir. Note this was not a factor in establishing soil clean up goals.	GW discharges to ditch.
Acme Solvent Reclaiming	Intermittent stream onsite.	Stream recharges aquifer.
Springfield Twp Dump	Adjacent wetlands	-
Fisher-Calo Chem	Adjacent wetlands	-
Wayne Waste Oil	In river floodplain. Wetlands onsite.	-
Pristine, Inc	None mentioned.	-
Oconomowoc Electroplating, Inc	Creek which hosts a fishery 500 ft to the south of site. Flows through wetlands.	GW discharges to creek.
Wausau Groundwater Contamination	River through site which encompasses city wellfield.	Under natural conditions groundwater flows to river. When city pumping, flow is to wells.
Metaltec-Aerosystem	Marshy wetland area SE of site.	-
Greenwood Chemical Site	Small creek 500' from boundary.	-
Tyson's Dump	SW runoffs and seeps contribute to offsite migration toward River. Site is bordered by tributaries to the river.	GW discharges to river.
Byron Barrel and Drum	Drainage ditches in neighboring farmfield drain to creek.	GW discharges to ditches.
Fulton Terminals	Bordered by a river.	-
American Thermostat	None mentioned.	-
Groveland Wells 1&2	In drainage basin of stream 450' to the east.	-
Waldick Aerospace Devices	None mentioned.	-
Caldwell Trucking	River which is source of municipal water is 4000' north site.	-
Bendix Flight System	Sits atop a topographic divide. Natural groundwater discharge into a wetlands east of site and headwaters of a creek west of the site.	-

(1) GW= groundwater in uppermost unconfined aquifer.

Table F-4: Summary of contaminant distribution.

Name	Area of contamination (ft ²)	Cause of contamination (1)	TCE Detected in: (2)			
			Soil	Ground-water (3)	Surface water	Air (4)
Main Street Wellfield	2.70E+04	SSL	Y	Y	N	ns
Zanesville Wellfield	1.50E+05	SSL, EXC	Y	Y	-	ns
Verona Wellfield	-	SSL, EXC, UST	Y	Y/Y	-	ns
Enviro-Chem	-	SSL	Y	Y	-	-
Acme Solvent Reclaiming	1.38E+05	SSL, EXC	Y	Y/N	ns	ns
Springfield Twp Dump	-	SSL, EXC	Y	Y/-	-	-
Fisher-Calo Chem	-	SSL, EXC	Y	Y	-	-
Wayne Waste Oil	-	SSL, EXC, UST	Y	Y	-	-
Pristine, Inc	1.20E+05	EXC	Y	Y/Y	-	ns
Oconomowoc Electroplating, Inc	-	SSL, EXC	Y	Y/Y/N	-	-
Wausau Groundwater Contamination	-	SSL, EXC	Y	Y	Y	ns
Metaltec-Aerosystem	-	SSL, EXC	Y	Y	-	-
Greenwood Chemical Site	5.50E+04	SSL, EXC	Y	Y	ns	ns
Tyson's Dump	-	SSL, EXC	Y	Y/ns	Y	N
Byron Barrel and Drum	5.63E+03	SSL, EXC, UST	Y	Y	N	ns
Fulton Terminals	7.85E+03	SSL	Y	Y	-	-
American Thermostat	3.00E+04	SSL	Y	Y/-	-	-
Groveland Wells 1&2	2.50E+04	SSL, UST, LF	Y	Y	Y	N
Waldick Aerospace Devices	-	SSL	Y	Y/-	-	-
Caldwell Trucking	-	EXC	Y	Y	-	-
Bendix Flight System	-	SSL, EXC	Y	Y/Y	Y	N

Notes:

1. SSL= surface spills and leaks, EXC= dumping in excavated areas includes buried drums, UST=leaking underground storage tank, LF=leach field
2. TCE detected in site characterization studies. Y= medium sampled and TCE detected, N=medium sampled and TCE not detected, ns= medium not sampled, - = no information in documentation reviewed.
3. Detection in uppermost unconfined aquifer. Where a deeper aquifer(s) is exists, detection in each successive aquifer. See Table F-2.

Table F-6: Summary of soil cleanup levels established.

Site Name	EPA		Basis for TCE Soil Clean up levels (1)			
	St	Reg	Calculated levels		Established levels	
			GW goal	Model used	Based on	(ppb)
Main Street Wellfield	IN	5	10-5 risk	Summers	Calculated	100
Zanesville Wellfield	OH	5	MCL	Summers	Calculated	6.3
Verona Wellfield	MI	5	na	na	MI goal	60
Enviro-Chem	IN	5	MCL	Summers	Calculated	240
Acme Solvent Reclaiming	IL	5	10-6 risk	HELP/Summers	Calculated	16 (4)
Springfield Twp Dump	MI	5	na	na	MI goal	60
Fisher-Calo Chem	IN	5	MCL	TBD	Calculated	-
Wayne Waste Oil	IN	5	MCL	TBD	Calculated	-
Pristine, Inc	OH	5	MCL	Summers	Calculated	175
Oconomowoc Electroplating, Inc	WI	5	WI Std	TBD	Calculated	-
Wausau Groundwater Cont.	WI	5	WI Std	Summers	Det Limit	10
Metaltec-Aerosystem	NJ	2	MCL	Eq. Partitioning	Calculated	5
Greenwood Chemical Site	VA	3	MCL	Summers	Calculated	130
Tyson's Dump	PA	3	na	na	CA	50
Byron Barrel and Drum	NY	2	MCL	Summers	Calculated	47
Fulton Terminals	NY	2	MCL	Summers	Calculated	2000
American Thermostat	NY	2	MCL	Multimed	Calculated	400
Groveland Wells 1&2	MA	1	-	Eq. Partitioning	Calculated	6
Waldick Aerospace Devices	NJ	2	na	na	NJ goal	1000
Caldwell Trucking	NJ	2	na	na	NJ goal	1000
Bendix Flight System	PA	3	1 ppb by CA	((2)	Calculated	100 (3)

Notes:

(1) MCL = maximum contaminant limit, - = not discussed in documentation reviewed CA = consent agreement between PRP and EPA, WI Std = Wisconsin standard for groundwater, TBD=to be determined in design phase

(2) An dilution factor of 100 is assumed between the soil pore water concentration in unsaturated zone and the bedrock aquifer where the GW goal is to be achieved.

(3) Limit for leachable VOCs (defined as soil pore water concentration) in the unsaturated zone.

(4) 16 ppb if a soil cap is used, and 140 ppb if a RCRA cap is placed on the site.

Table F-7: Summary of remediation strategies.

Name	Soil Remedy for TCE (1)	Other Remedy for TCE (2)
Main Street Wellfield	ISVE in one area; Exc/Incin in another.	GWCT (send to city's potable water system); DR
Zanesville Wellfield	ISVE	GWCT
Verona Wellfield	ISVE	GWCT
Enviro-Chem	ISVE enhanced by RCRA cap.	Contingent remedy of GWCT if cleanup stds are not met, DR
Acme Solvent Reclaiming	Exc/Treatment by LTTS and ISVE. RCRA cap or soil cover depending on cleanup levels achieved.	Incineration of liquid and sludges remaining onsite. GWCT (discharge to SW). Provide alternate water supply.
Springfield Twp Dump	Exc/Incin and ISVE of soils at depth.	GWCT (reinjection to aquifer); recontouring of excavated areas and control of ash or dust emissions.
Fisher-Calo Chem	Exc and Soil flushing or ISVE.	Fencing, GWCT w/ reinjection into aquifer to flush contaminants from soil and gw.
Wayne Waste Oil	ISVE	Security fence, DR, GWCT, tank contents removed and treated.
Pristine, Inc	Exc/Incin of soils to 1'. ISVE of soils 1'-12'. Use of ISVE to dewater the upper aquifer.	Fence. Deed restrictions. Add itional GW investigation to delineate lower aquifer contamination to design and construct GWCT.
Oconomowoc Electroplating, Inc	Exc and offsite treatment and disposal.	GWCT discharge to creek.
Wausau Groundwater Contamination	ISVE	GWCT using municipal wells and existing air strippers.
Metaltec-Aerosystem	Exc. Treatment via heat addition. Offsite disposal.	Supplemental RI/FS for gw contamination. Alternative water supply.
Greenwood Chemical Site	Exc of soil. Staging and screening. Incineration.	OU-2 will address additional soil, gw, and sediment contamination.
Tyson's Dump	ISVE	Leachate (seep/spring) collection and treatment.
Byron Barrel and Drum	In situ flushing	GWCT with reinjection to the aquifer in contaminated areas and discharge of excess to sw.
Fulton Terminals	Exc/treatment via low-temp thermal extraction/ replacement.	GWCT, w/ reinjection to aquifer.
American Thermostat	Exc/ Trt using low-temp enhanced volatilization/replacement.	GWCT, w/ reinjection to aquifer.
Groveland Wells 1&2	ISVE	GWCT w/ recharge to aquifer.
Waldick Aerospace Devices	In-situ air stripping or Exc	Installation of add'l gw wells, access and well restrictions.
Caldwell Trucking	Exc. Trtmt via ht addition. Disp of untreated soil and waste in secure landfill.	Treatment of GW from municipal water supply well.
Bendix Flight System	ISVE and soil aeration.	GWCT on site and treatment of water at each affected residential well.

Notes:

(1) ISVE=in-situ vapor extraction, Exc=excavation, Incin=incineration, LTTS=low-temperature thermal stripping

(2) GWCT=groundwater collection and treatment, DR=deed restrictions until goals are met, SW=surface water, OU=operable unit, GW= groundwater.

APPENDIX G:
EFFECTIVE HALF LIVES OF BENZENE, TCE, CHLORDANE,
AND BAP: A LITERATURE REVIEW

INTRODUCTION

In SoilRisk, τ and τ_{sat} (day) are the effective half-lives of the chemical contaminant due to biological/chemical degradation in the unsaturated and the saturated zones, respectively. They represent half-lives due to the most important degradation process, whether it is aerobic or anaerobic biodegradation or an abiotic process such as hydrolysis. Overall effective degradation is assumed first-order and the reaction rate in the unsaturated zone, μ (day^{-1}) is calculated in the model by $\ln(2)/\tau$. The reaction rate in the saturated zone, μ_{sat} (day^{-1}) is calculated using the same relationship with τ_{sat} in the denominator.

In assigning values to the effective half-lives for Benzene, Trichloroethylene (TCE), Chlordane, and Benzo[a]pyrene (BAP) in (Labieniec et al., 1994), Table 2, it was assumed that aerobic conditions prevail in both the saturated and unsaturated zones. This is a common assumption for the unsaturated zone (e.g., (Howard et al., 1991; Ostendorf et al., 1991; Wilson et al., 1981)). The assumption that the saturated zone maintains aerobic conditions is based on the fact that the saturated zone is also assumed unconfined and shallow. Thus, the possible degradation reactions that are relevant are aerobic biodegradation and abiotic degradation.

Even with these simplifying assumptions, it is known that degradation rates are sensitive to such site conditions as temperature, pH, the prescience of other substrates that may serve as co-metabolites, and the microbial population present and its nutrient status. Since the purpose of this effort was not to model the influence of site conditions on the degradation half-life, reasonable values were assigned to τ and τ_{sat} for the assumed site conditions based on values reported in the literature from laboratory or field studies. The studies reviewed are summarized here.

BENZENE

The effective half-life of 15 days for benzene in soil and groundwater was estimated based on the range of measurements of total benzene biodegradation in dilute aqueous solution under aerobic conditions in the laboratory. Chiang et al. (1988) measured a biodegradation half-life of 5-20 days using laboratory microcosms consisting of subsoil and groundwater (0.12 to 16 g/m³ total benzene) from a hydrocarbon contaminated site. They found the degradation rates to be similar for cores taken from the vadose and saturated zones.

Vaishnav et al. (1987), incubated natural groundwater spiked with benzene (<4 g/m³) and obtained a biodegradation half-life estimate of 28 days. (Karlson et al., 1989) obtained a half-life for benzene of about 2 days by incubating a petroleum contaminated groundwater sample (6.2 g/m³ benzene).

TCE

The extremely long effective half-life for TCE of 4.7×10^8 was established based on the half life for abiotic hydrolysis. A recent study found that TCE was not degraded by indigenous bacteria under aerobic conditions. Fan et al. (1993) measured the biodegradation of TCE in dilute aqueous solution (0.1-1 g/m³ TCE) by indigenous microbial populations in three unsaturated soils incubated under aerobic conditions. TCE was not degraded in any of the soils unless a co-substrate, toluene, was present. Similarly, Wilson et al. (1981), using a sandy soil as the biological seed and TCE in dilute aqueous solution, found no significant degradation of TCE under aerobic conditions unless the bacteria were exposed to methane. It should be noted that two other studies have detected microbial degradation under aerobic conditions using indigenous microbial populations (McClellan et al., 1989; Walton et al., 1990), but Fan and Scow (1993) point to the possibility of the presence of undetected co-substrates as an explanation for the discrepancy. With regard to abiotic processes, Jeffers et al. (1989) have measured the abiotic half life for TCE in dilute aqueous solution due to hydrolysis. At ambient temperature and neutral pH, it is estimated to be 4.7×10^8 days.

Since there is no evidence of any significant biodegradation of TCE under aerobic conditions, it was assumed that hydrolysis is the dominant mechanism of loss of TCE due to reaction.

CHLORDANE

The chlordane effective half-lives are based on the results of a survey of sites contaminated with technical-grade chlordane and protected from water deposition and erosion performed by Puri et al.(1990). (Technical grade chlordane is a mixture of variously chlorinated compounds including pure chlordane.) They found that after 7 years, more than 70% of the originally applied chlordane could be recovered. Additionally, chromatographic analysis revealed that profiles of the residues were almost identical to the original formulation. Assuming first order degradation, this translates into roughly a 5000 day half life. The relative recalcitrance of chlordane in the field is supported by the laboratory studies by Tabak et al. (1981) where no degradation of chlordane was detected when a chlordane spiked dilute aqueous solution ($<10 \text{ g/m}^3$) was incubated in the dark for 28 days using a settled domestic waste water as the inoculum.

BAP

The effective half life for BAP of 300 days is based on the range of half lives (178-462 days) reported by Sims et al. (1988) for aqueous aerobic biodegradation in the laboratory. The reported half-lives were corrected for volatilization losses. Studies were performed in soil:water microcosms using two types of sandy loam soil. Pure chemical was applied at 33mg/kg to 250 g of air dried soil at -0.33 bar moisture, conditions under which undissolved BAP was certainly present. However, the 300 day half-life used is also within the range reported for aqueous aerobic degradation given by Howard et al. (1991). No distinction was made by Sims et al. (1988) between complete degradation and transformation into intermediate products. It should be noted that half-lives to attain

complete mineralization can be significantly longer. Heitkamp et al.(1987) measured the microbial mineralization of BAP in sediment: water microcosms under aerobic conditions and obtained half-lives ranging from 1400 days when the sediment was sampled from an ecosystem known to have chronic exposure to polynuclear aromatic hydrocarbons to not-detectable when the sediment was taken from a pristine ecosystem.

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APPENDIX H:
SITE-SPECIFIC SENSITIVITY ANALYSIS PLOTS

A parametric sensitivity analysis was performed to determine the influence of SoilRisk site input parameters on the total unit risk estimate and the unit risk estimate contributed by each of the exposure routes. The results are summarized in Chapter 2 and presented in full here. Each site parameter was varied individually over ranges appropriate for the generalized site described in Chapter 2 while all other site parameters were held at a median point value (Chapter 2, Table 4). Parameter values characterizing the generalized site are summarized in Chapter 2, Table 1. Preliminary model runs indicated that the unit risk due to the inhalation of dust mobilized from the site was insignificant relative to all other exposure routes for all exposure scenarios. Therefore, the parameters required by the dust module of SoilRisk were not varied in the sensitivity and were held at the conservative values presented in Chapter 2, Table 5.

Results are presented here in the form of a series of plots of unit risk (total risk and risk due to each exposure route in each exposure scenario (Table H-1)) versus each parameter of interest. Detailed descriptions of the exposure scenarios and exposure routes can be found in Chapter 1. Results for the offsite residential exposure scenario are presented in Figures H-1 to H-4; for the onsite residential exposure scenario, in Figures H-5 to H-8; for the recreational exposure scenario, in Figures H-9 to H-12; and for the commercial/industrial exposure scenario, in Figures H-13 to H-16. Refer to Figure 3 in Chapter 2 for an overview of the relative importance of each exposure route for each exposure scenario.

Table H-1: Exposure routes considered for each exposure scenario†

Symbol	Description	Exposure Scenario†			
		Res-on	Res-off	Rec	Com
pw	Ingestion of potable groundwater	✓	✓	✓	✓
si	Ingestion of site soil	✓		✓	✓
derm	Dermal absorption	✓		✓	✓
	Inhalation of vapors contaminated by:				
air	(i) volatilization from site surface	✓	✓	✓	✓
nc	(ii) non-consumptive use of water	✓	✓		
sg	(iii) infiltration of soil-gas into house	✓			
dust	Inhalation of dust mobilized from site	✓		✓	✓

† Res-on=onsite residential, Res-off=offsite (100m) residential, Rec=recreational, and Com= commercial/industrial.

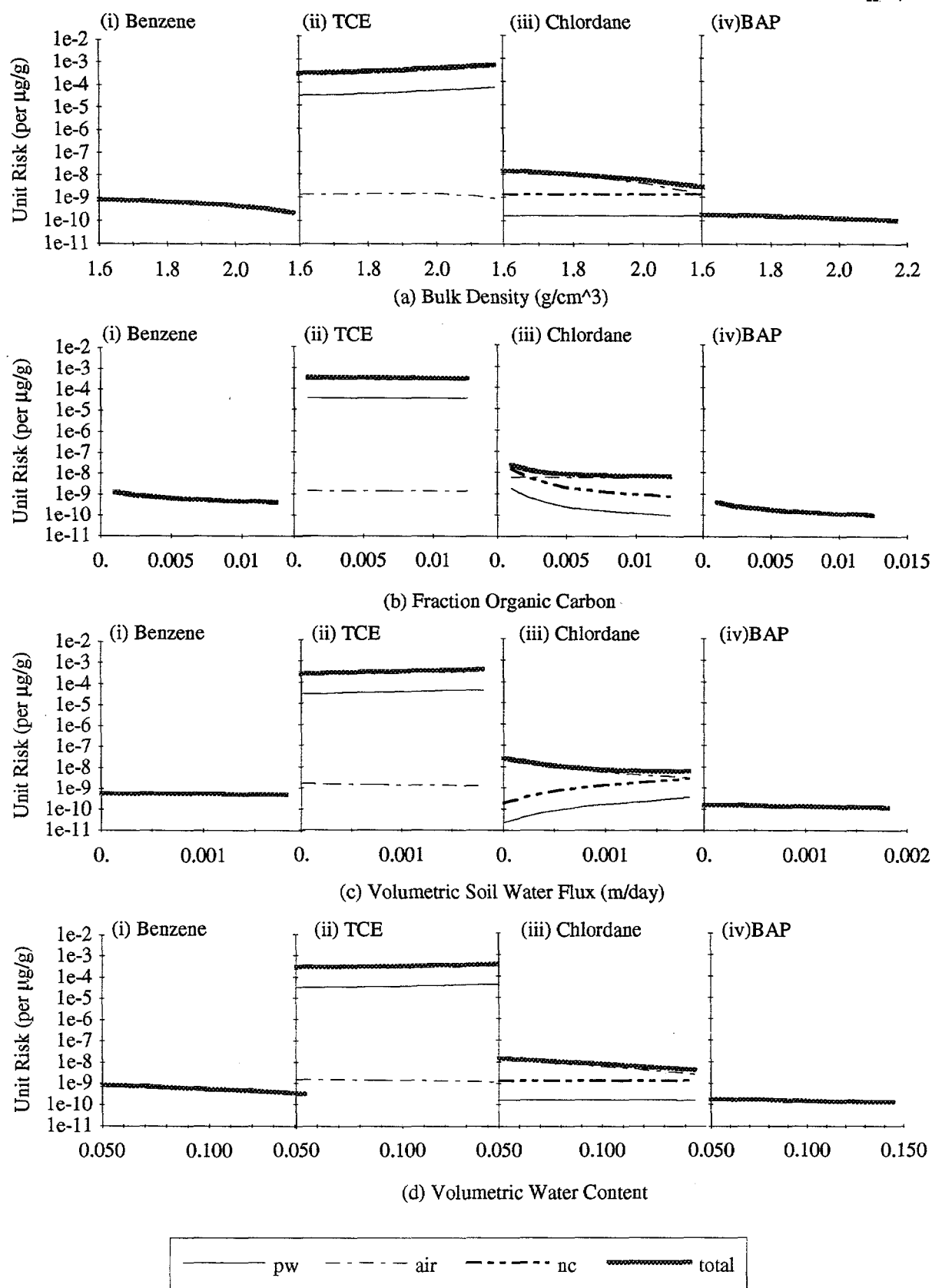


Figure H-1: Sensitivity of OFFSITE RESIDENTIAL (100m) SoilRisk risk estimates (total and due to each exposure route) to UNSATURATED zone parameters (a) bulk density, (b) fraction organic carbon, (c) volumetric soil water flux, and (d) volumetric water content for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

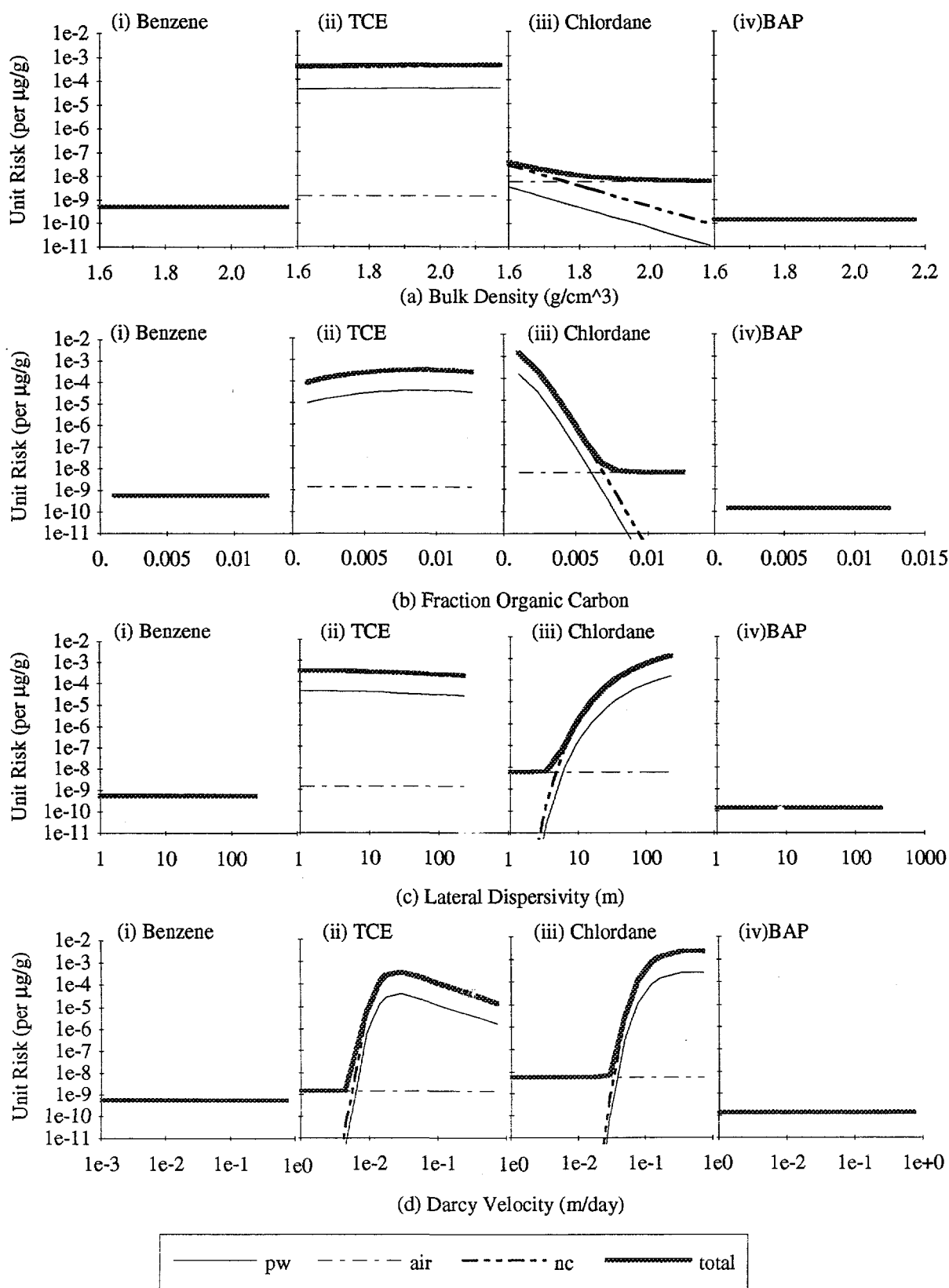


Figure H-2: Sensitivity of OFFSITE RESIDENTIAL (100m) SoilRisk risk estimates (total and due to each exposure route) to SATURATED zone parameters (a) bulk density, (b) fraction organic carbon, (c) lateral dispersivity, and (d) Darcy velocity for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

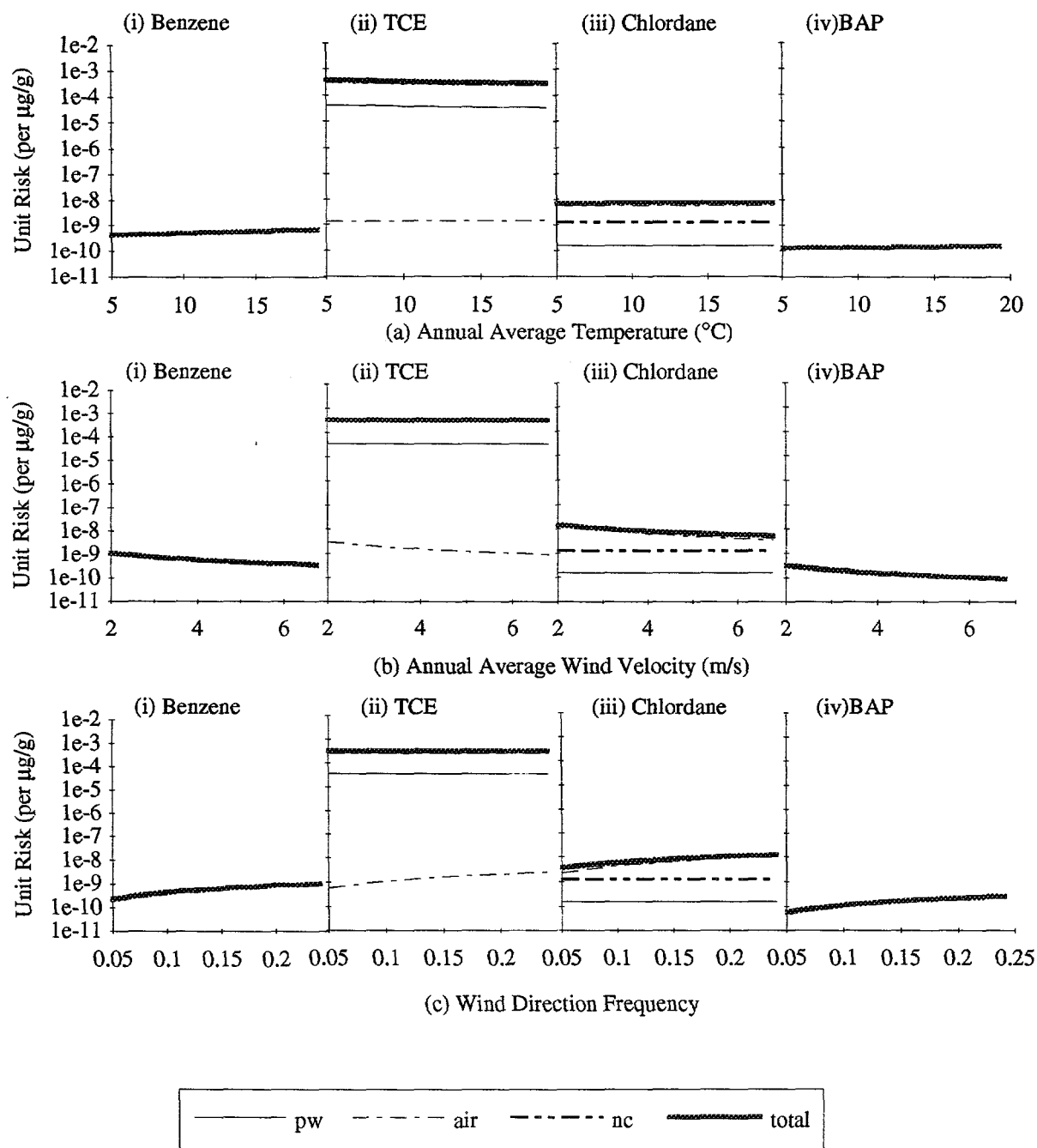
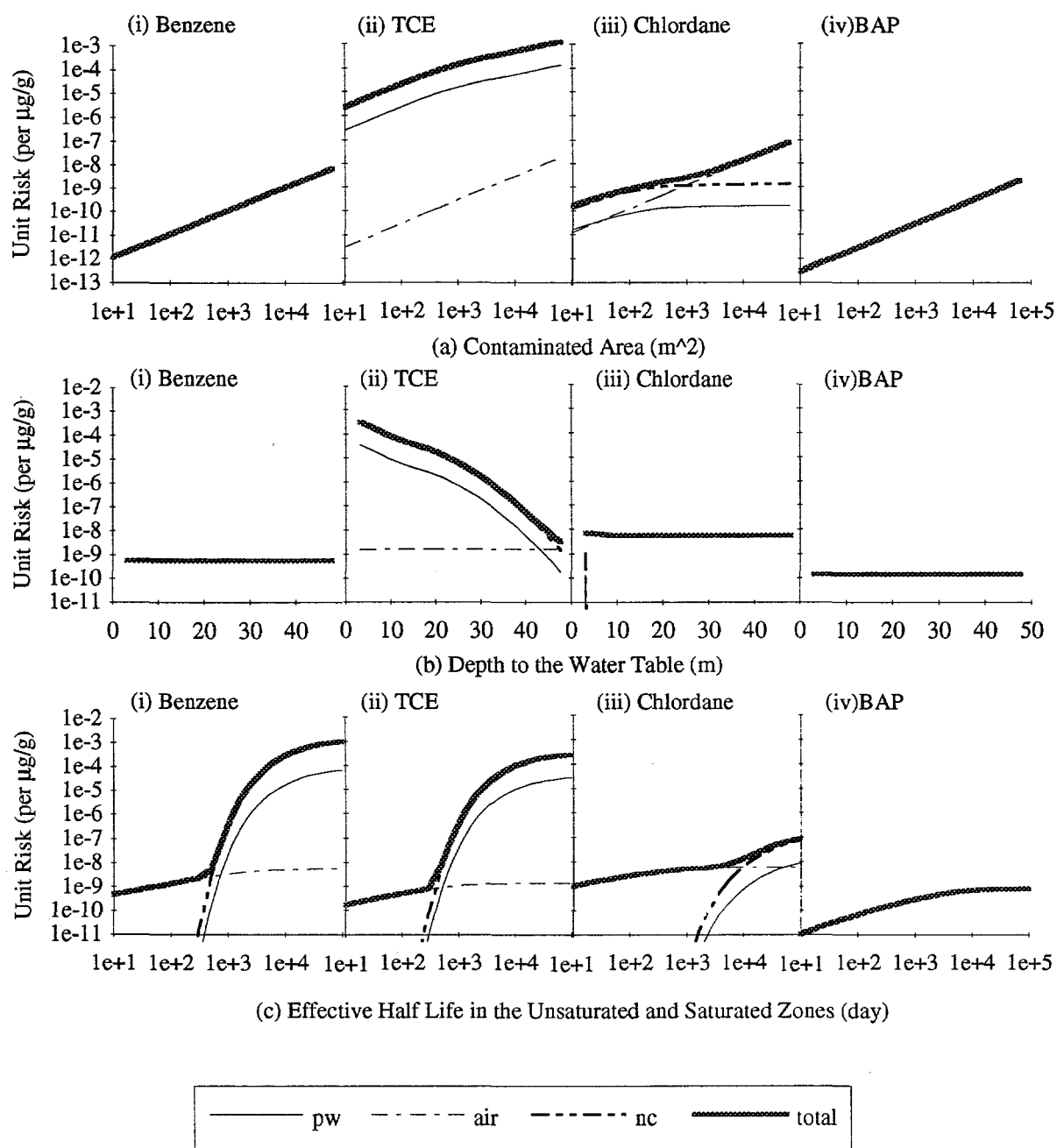


Figure H-3: Sensitivity of OFFSITE RESIDENTIAL (100m) SoilRisk risk estimates (total and due to each exposure route) to CLIMATIC parameters (a) annual average air temperature, (b) surface wind velocity, and (c) wind direction frequency for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.



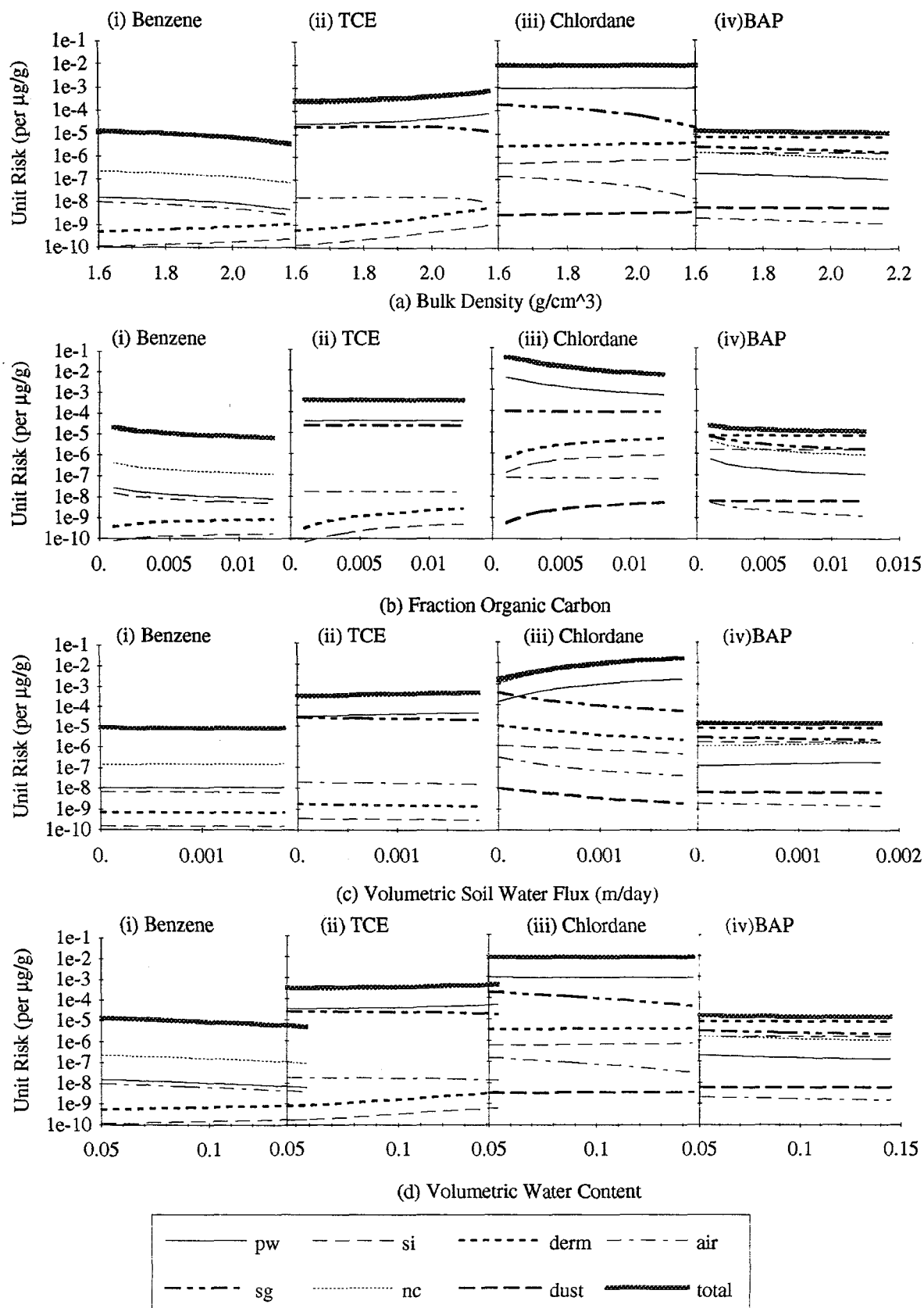


Figure H-5: Sensitivity of ONSITE RESIDENTIAL SoilRisk risk estimates (total and due to each exposure route) to UNSATURATED zone parameters (a) bulk density, (b) fraction organic carbon, (c) volumetric soil water flux, and (d) volumetric water content for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

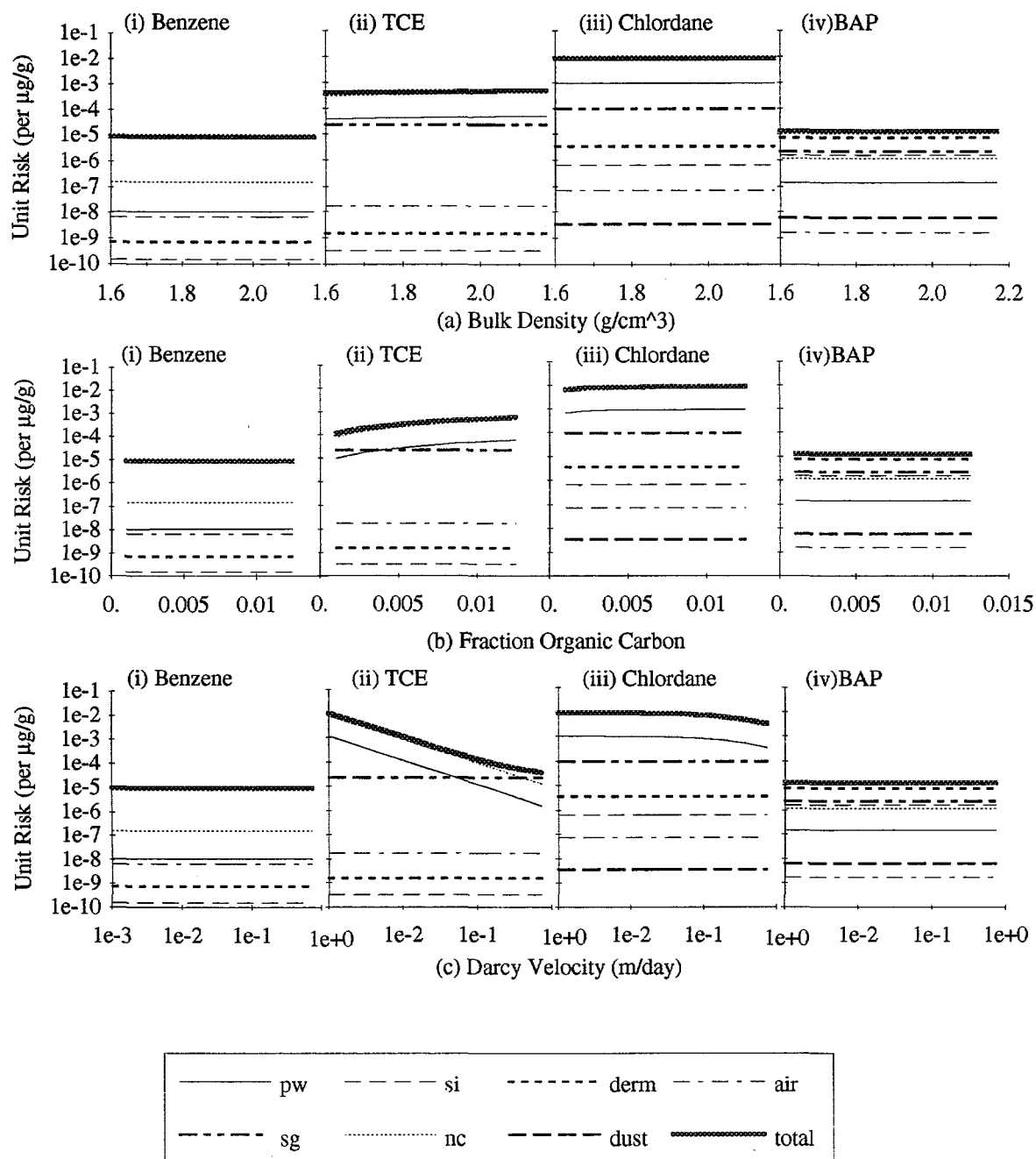


Figure H-6: Sensitivity of ONSITE RESIDENTIAL SoilRisk risk estimates (total and due to each exposure route) to SATURATED zone parameters (a) bulk density, (b) fraction organic carbon, and (c) Darcy velocity for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

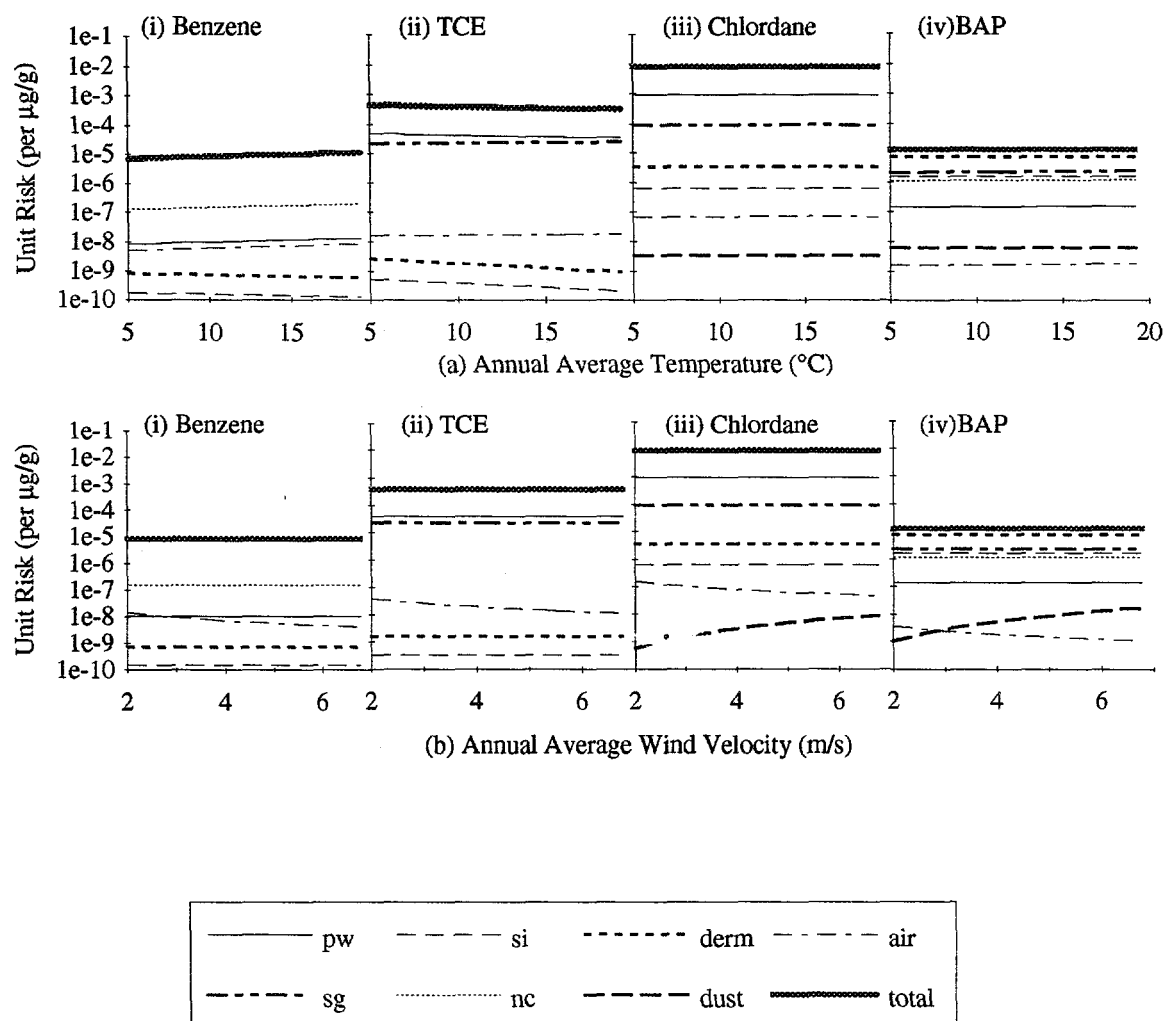


Figure H-7: Sensitivity of ONSITE RESIDENTIAL SoilRisk risk estimates (total and due to each exposure route) to CLIMATIC parameters annual average (a) air temperature and (b) surface wind velocity for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

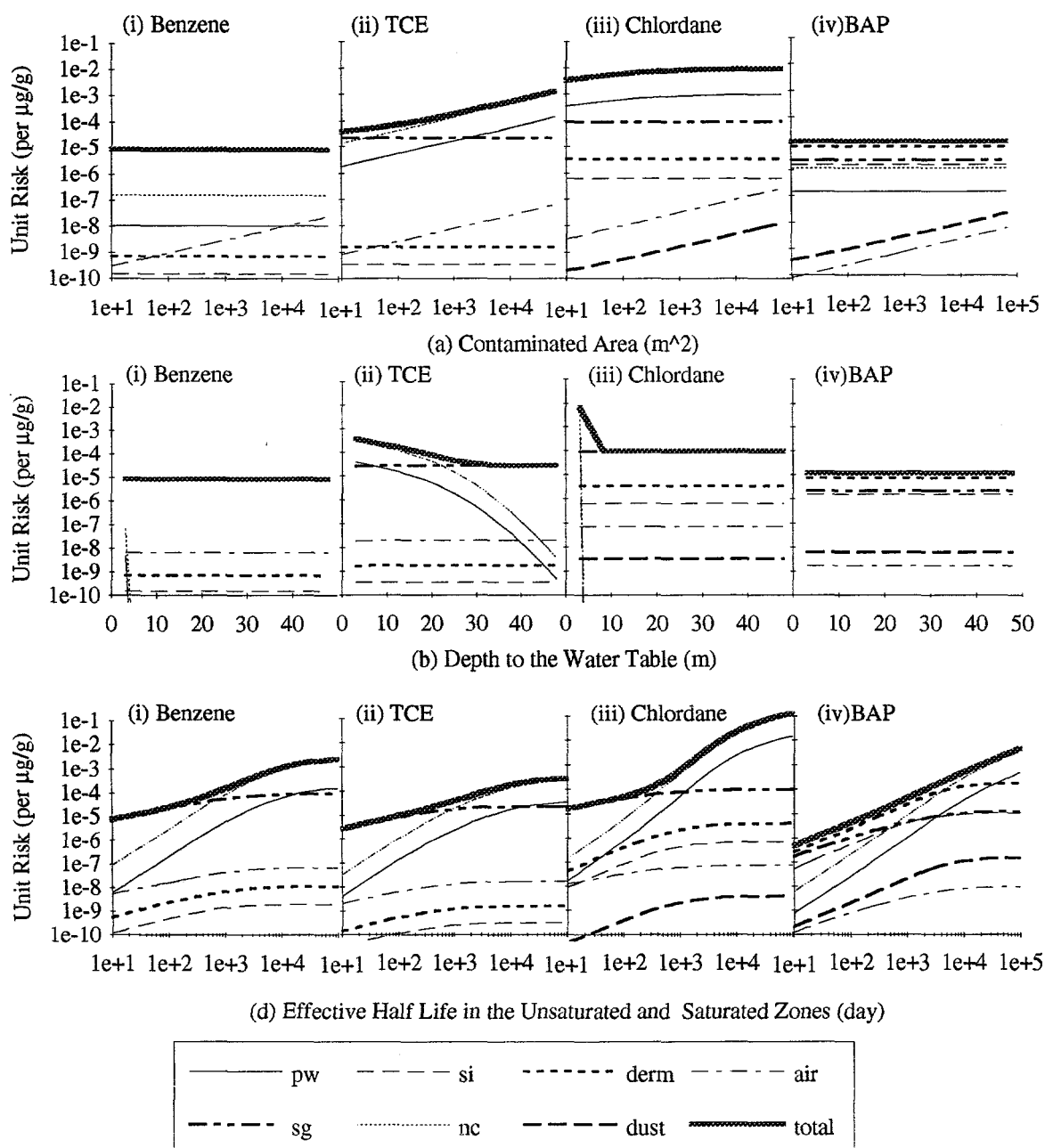


Figure H-8: Sensitivity of ONSITE RESIDENTIAL SoilRisk risk estimates (total and due to each exposure route) to SITE DIMENSIONS, (a) area and (b) depth to water table, and (c) EFFECTIVE HALF LIFE IN THE UNSATURATED AND SATURATED ZONES for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

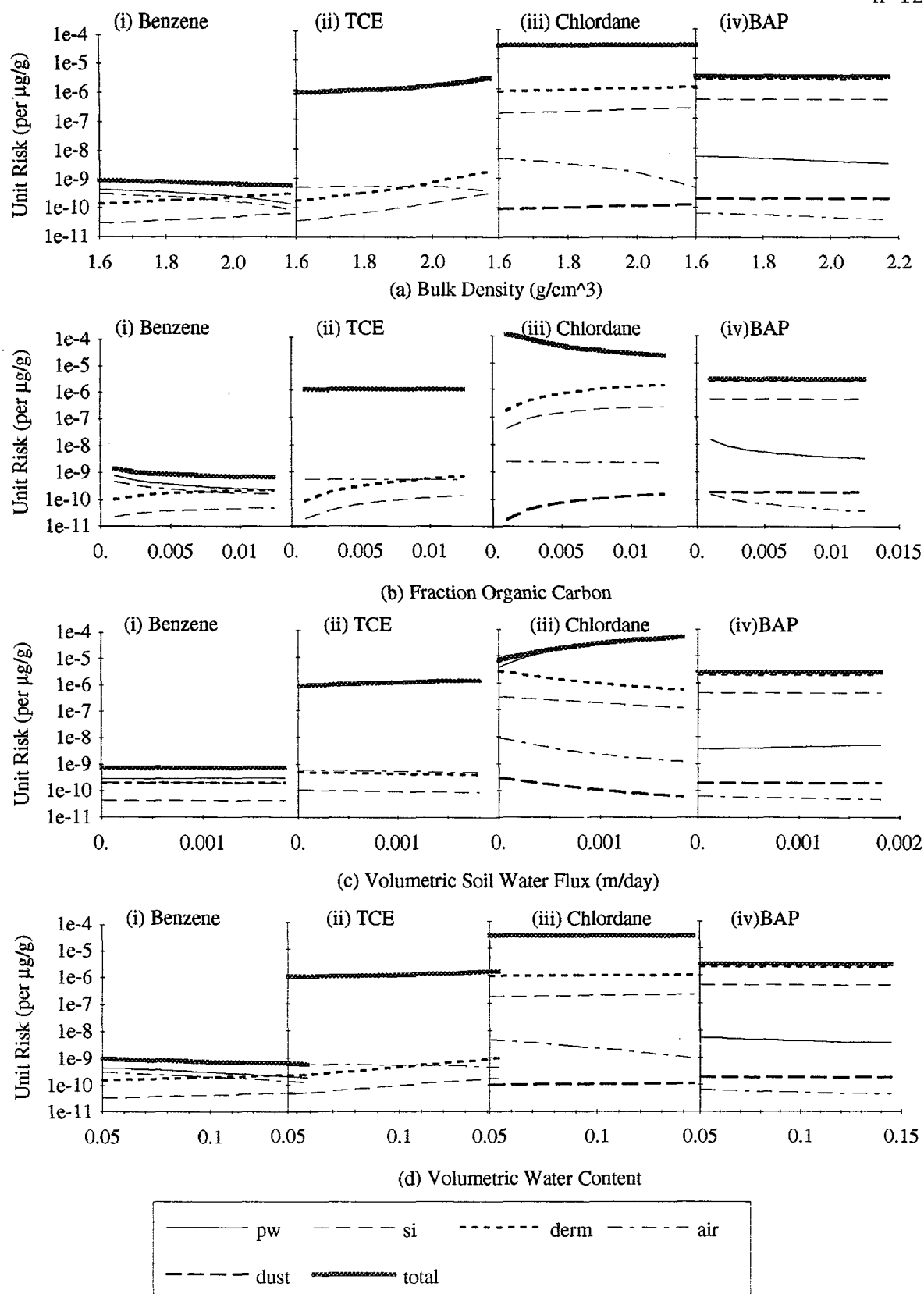


Figure H-9: Sensitivity of RECREATIONAL SoilRisk risk estimates (total and due to each exposure route) to UNSATURATED zone parameters (a) bulk density, (b) fraction organic carbon, (c) volumetric soil water flux, and (d) volumetric water content for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

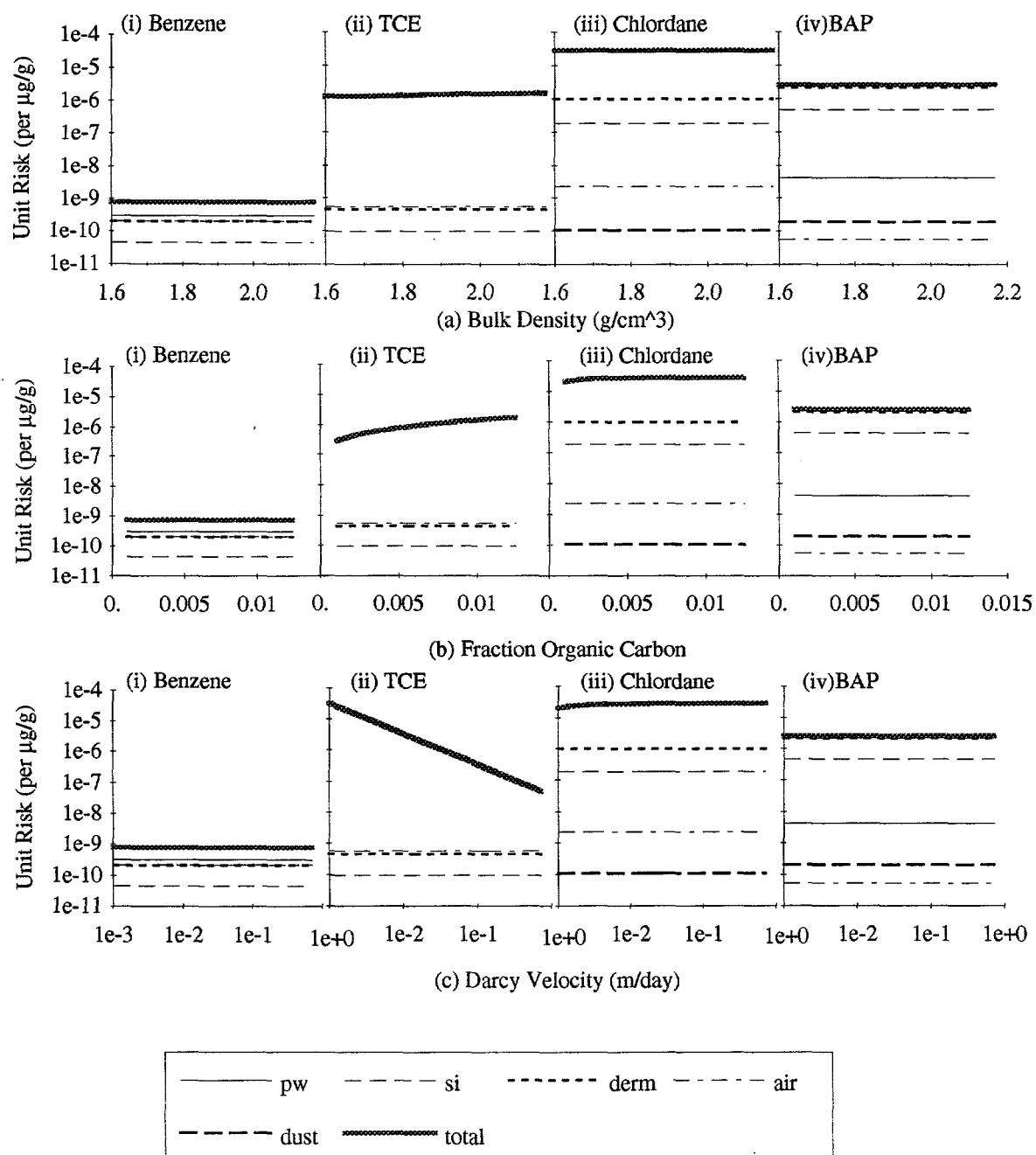


Figure H-10: Sensitivity of RECREATIONAL SoilRisk risk estimates (total and due to each exposure route) to SATURATED zone parameters (a) bulk density, (b) fraction organic carbon, and (c) Darcy velocity for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

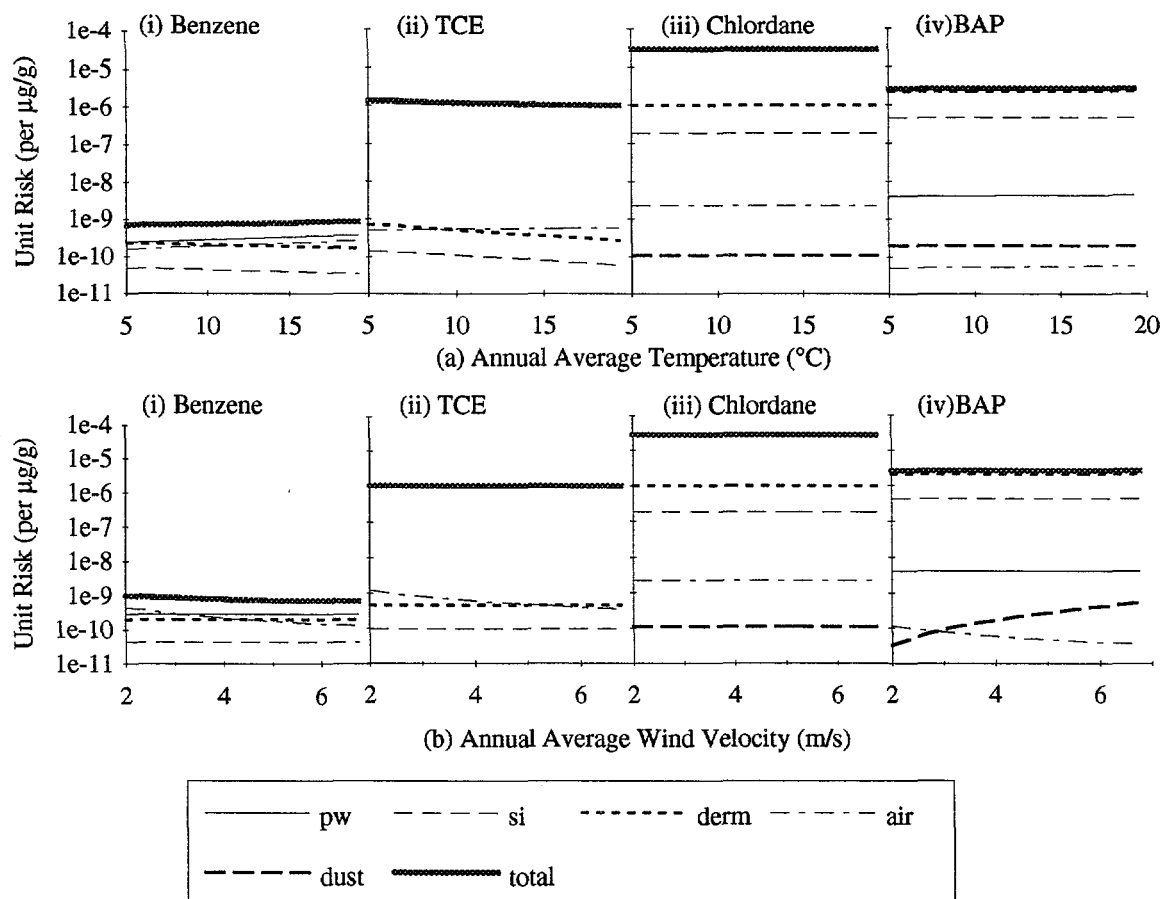


Figure H-11: Sensitivity of RECREATIONAL SoilRisk risk estimates (total and due to each exposure route) to CLIMATIC parameters (a) annual average air temperature and (b) surface wind velocity for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

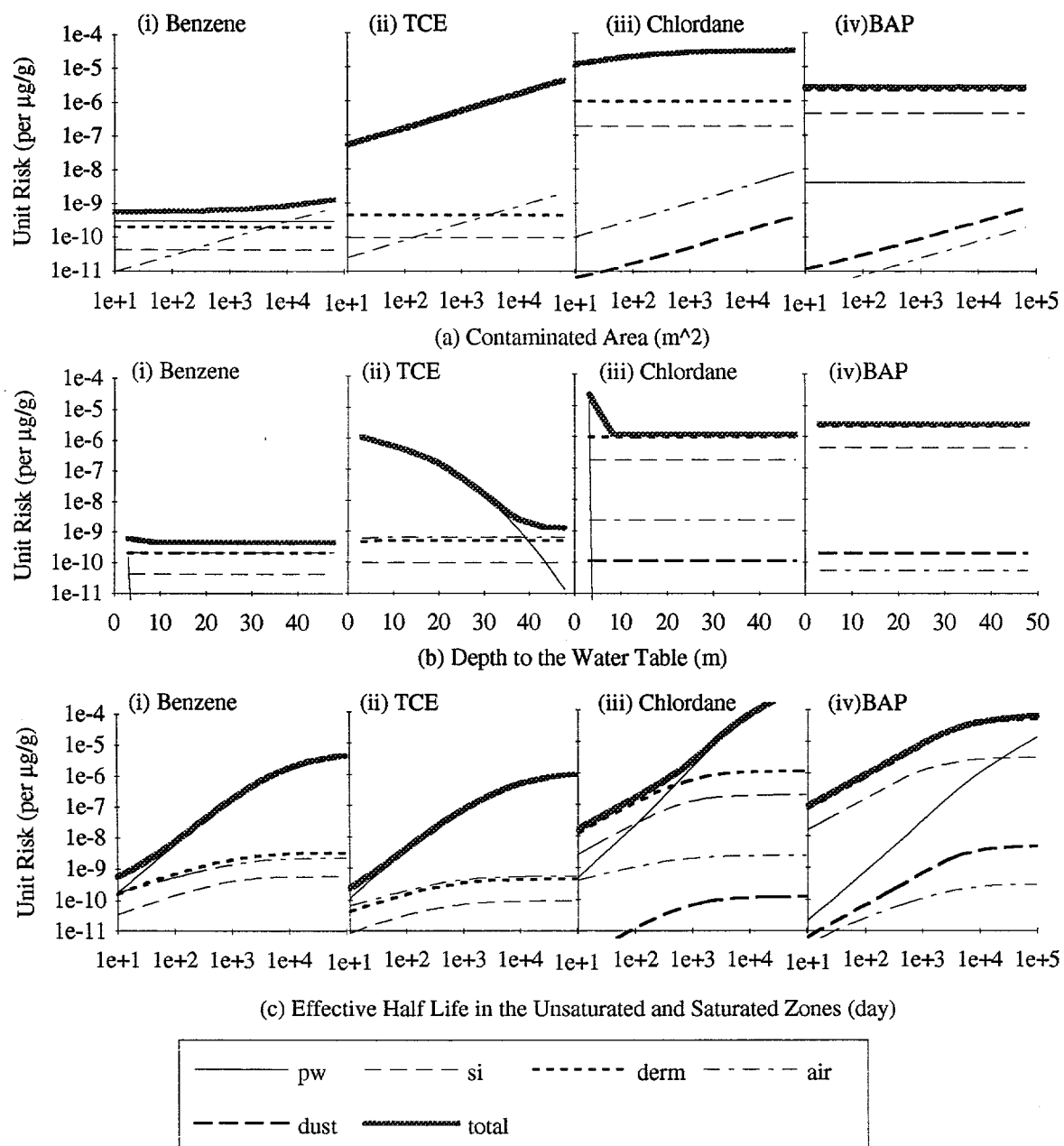


Figure H-12: Sensitivity of RECREATIONAL SoilRisk risk estimates (total and due to each exposure route) to SITE DIMENSIONS, (a) area and (b) depth to water table, and (c) EFFECTIVE HALF LIFE IN THE UNSATURATED AND SATURATED ZONES for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

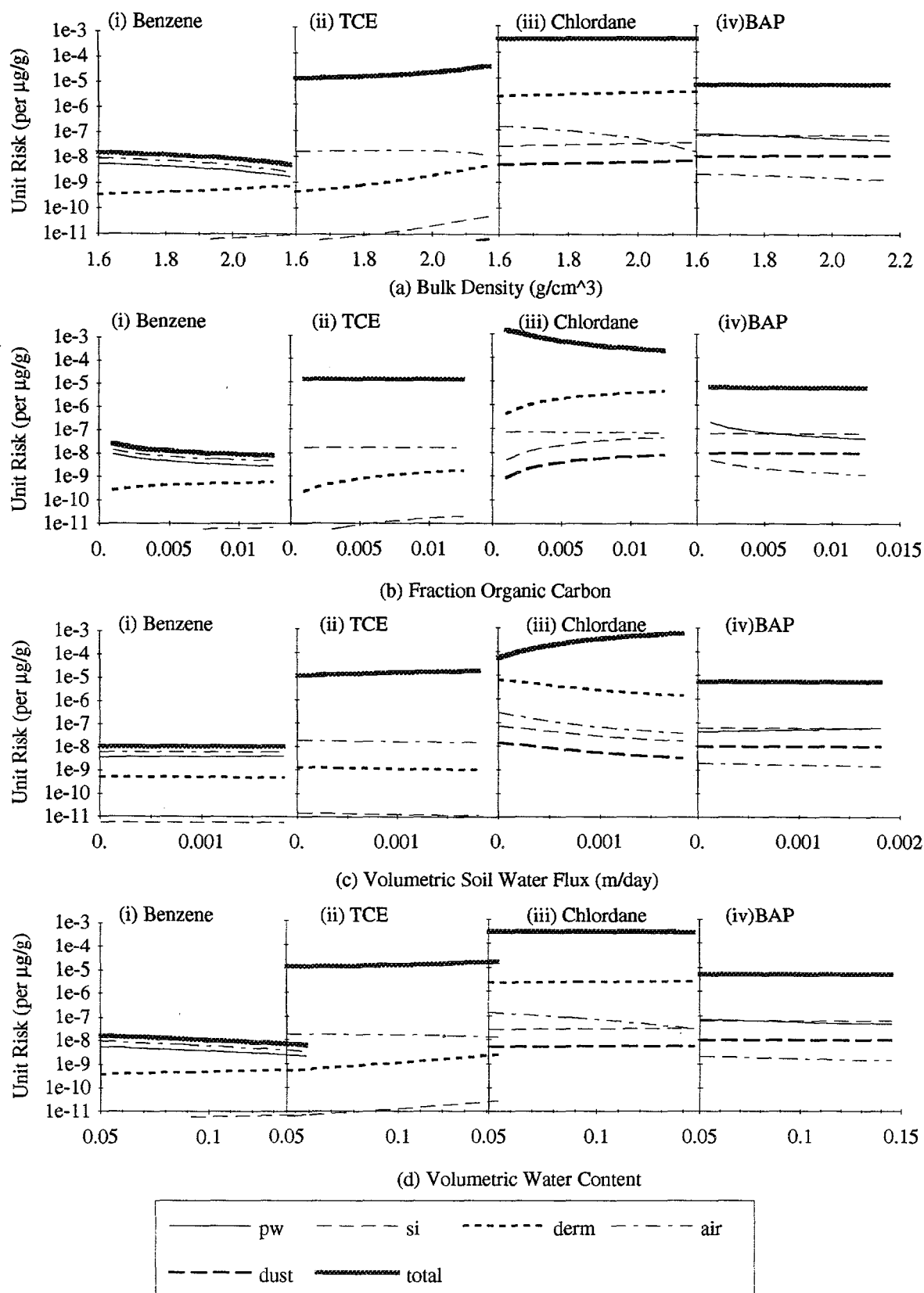


Figure H-13: Sensitivity of COMMERCIAL/INDUSTRIAL SoilRisk risk estimates (total and due to each exposure route) to UNSATURATED zone parameters (a) bulk density, (b) fraction organic carbon, (c) volumetric soil water flux, and (d) volumetric water content for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

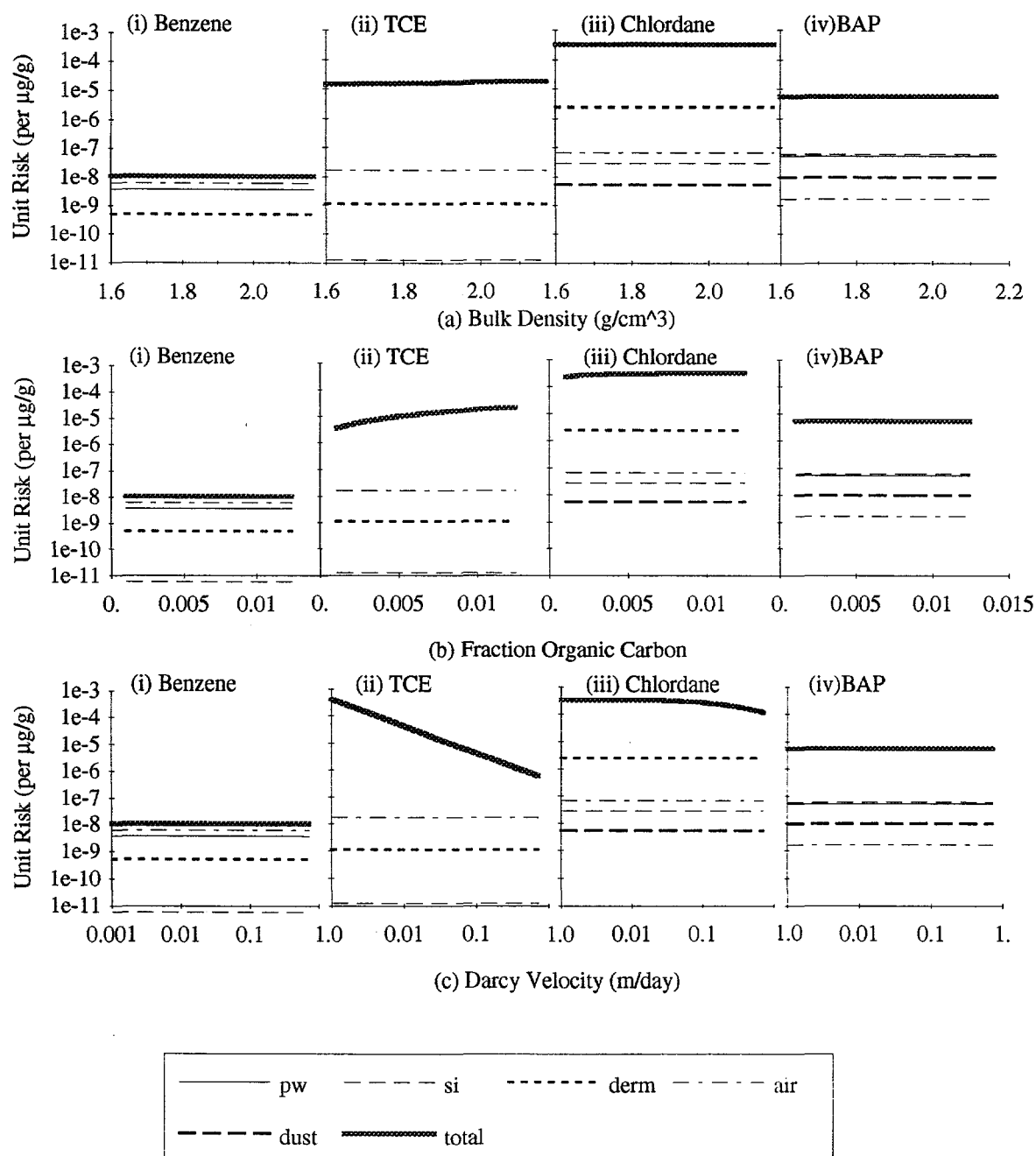


Figure H-14: Sensitivity of COMMERCIAL/INDUSTRIAL SoilRisk risk estimates (total and due to each exposure route) to SATURATED zone parameters (a) bulk density, (b) fraction organic carbon, and (c) Darcy velocity for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

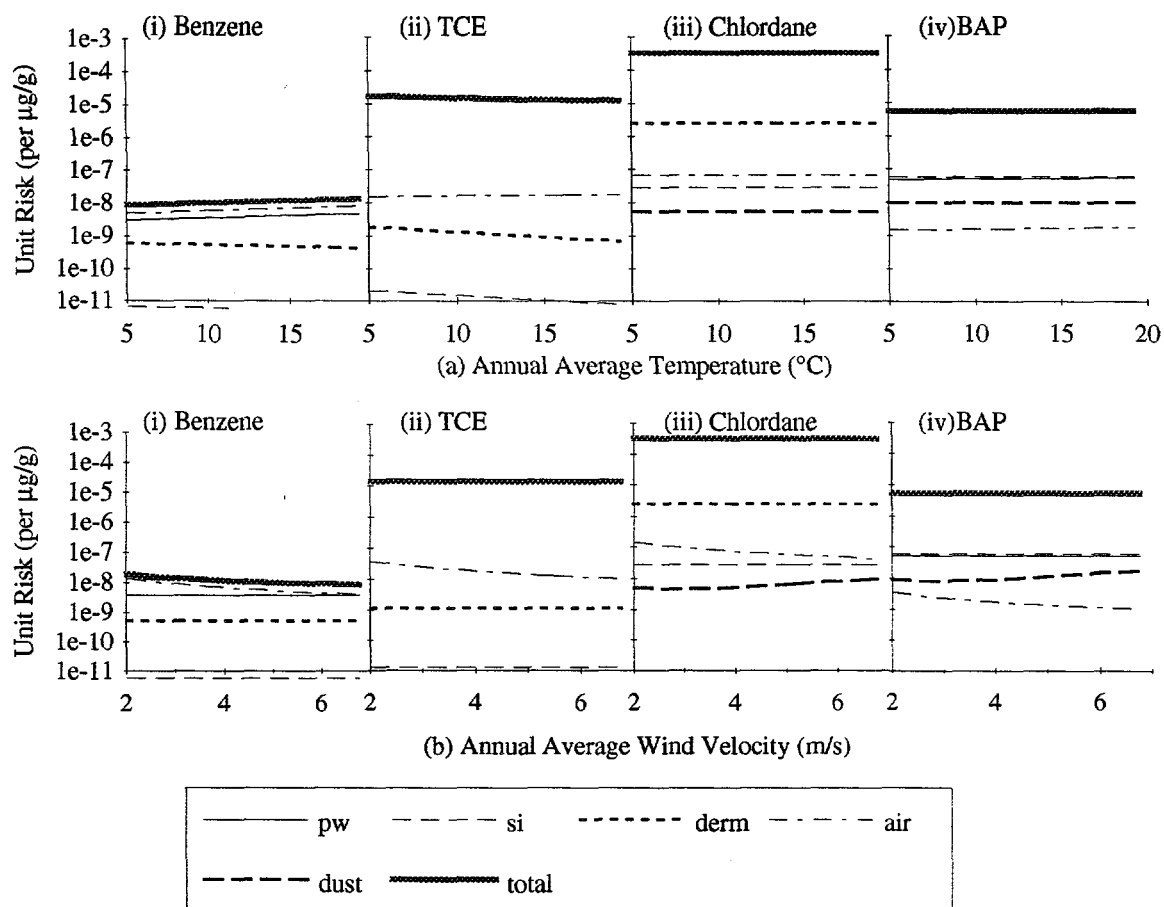


Figure H-15: Sensitivity of COMMERCIAL/INDUSTRIAL SoilRisk risk estimates (total and due to each exposure route) to CLIMATIC parameters (a) annual average air temperature and (b) surface wind velocity for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

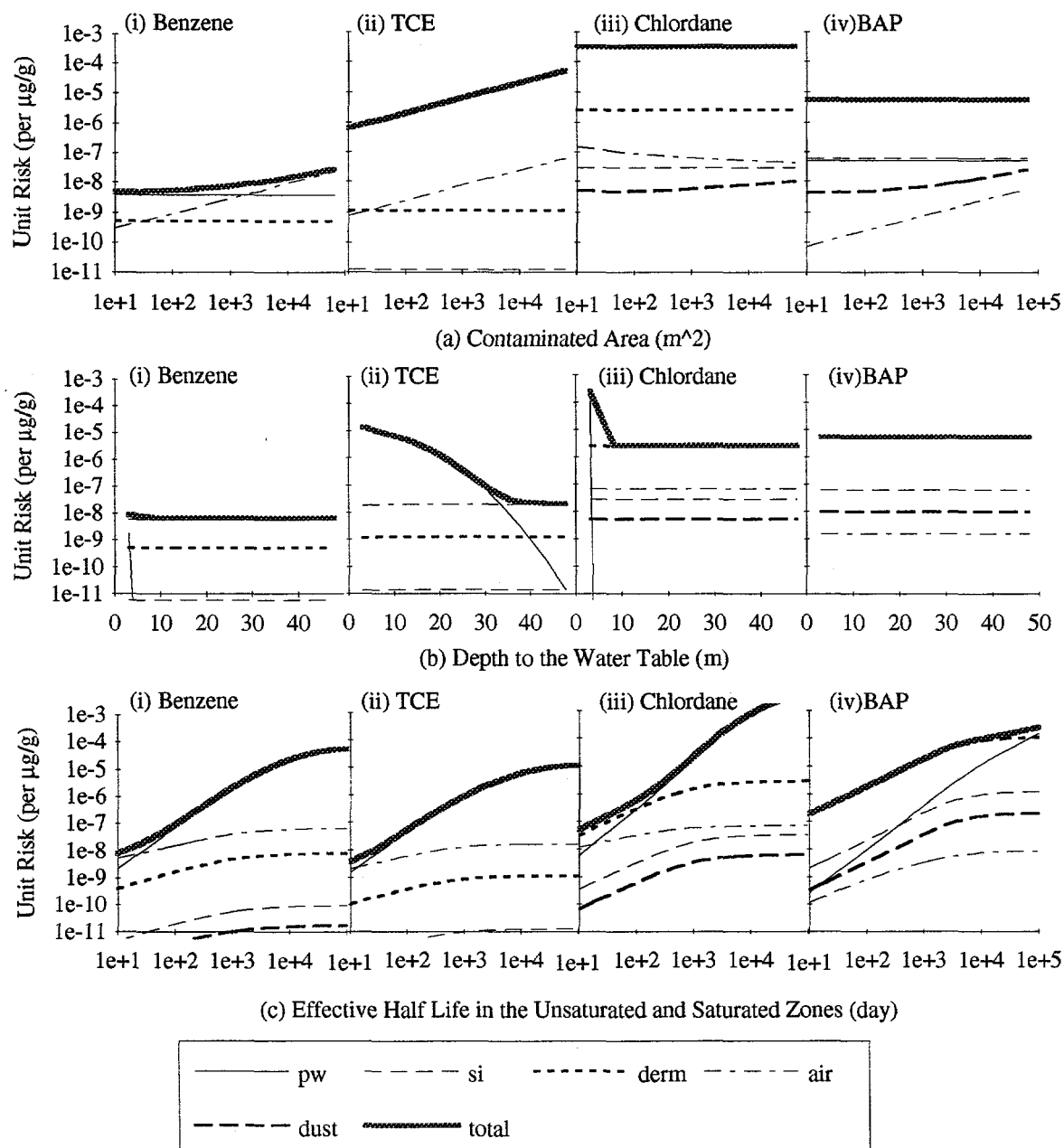


Figure H-16: Sensitivity of COMMERCIAL/INDUSTRIAL SoilRisk risk estimates (total and due to each exposure route) to SITE DIMENSIONS, (a) area and (b) depth to water table, and (c) EFFECTIVE HALF LIFE IN THE UNSATURATED AND SATURATED ZONES for (i) benzene-, (ii) TCE-, (iii) chlordane-, and (iv) BAP-contaminated soil. For a key to the exposure route symbols, see Table H-1.

APPENDIX I:
FREQUENCY HISTOGRAMS OF DRASTIC PARAMETERS
FOR ROSS COUNTY, OHIO

INTRODUCTION/ BACKGROUND

This appendix presents the area-weighted histograms of DRASTIC (Aller et al., 1985) parameters for Ross County, Ohio in Figures I-1 to I-22. The histograms were created using Frederick (1991) as described below and were used in assigning the probability distribution functions representing variability in hydrogeologic conditions across Ross County, Ohio (Chapter 3, Tables 1 and 4).

DRASTIC (Aller et al., 1985) is a methodology for mapping and ranking the groundwater pollution potential of the different hydrogeologic settings in an area. A hydrogeologic setting is defined as a mappable unit with common hydrogeologic characteristics. These characteristics include major geologic and hydrologic factors that affect and control groundwater movement. Specifically, the hydrogeologic characteristics considered in DRASTIC include depth to water, net recharge, topography, hydraulic conductivity of the aquifer, and the texture of the soil, vadose zone, and aquifer media. (In DRASTIC, soil is assumed to be the unconsolidated media from the surface to 1.8 m and the vadose zone is the consolidated or unconsolidated media from 1.8 m to the water table.) Hydrogeologic settings with similar characteristics have been grouped into the 15 different groundwater regions in the U.S. shown in Chapter 3, Figure 2 (Aller et al., 1985).

Ross County is in the center of the state of Ohio as shown in Chapter 3, Figure 3 and is primarily in the Glaciated Central Groundwater Region (Region 7 in Chapter 3, Figure 2). About 20% of the county is in the Non-Glaciated Central Groundwater Region (Region 6 in Chapter 3, Figure 2). Table I-1 presents a summary of the hydrogeologic settings found in Ross County and the number of sub-settings in each that were mapped in Frederick (1991). Four hydrogeologic settings were identified in Region 6, and 18 in Region 7. In

addition, three to 267 hydrogeologic sub-settings were mapped within each hydrogeologic setting. The total area taken up by each hydrogeological setting is also given in Table I-1.

DEVELOPMENT OF AREA-WEIGHTED HISTOGRAMS

In this work, the area of each hydrogeologic sub-setting in Ross County, Ohio was measured using a planimeter and the map provided in Frederick (1991). Each hydrogeologic sub-setting is described in Frederick (1991) by a range of values for depth to water, net recharge, and hydraulic conductivity, and by a general description of the soil, vadose, and aquifer media. The ranges used for depth to water, net recharge, and hydraulic conductivity are standardized and are summarized in Table I-2. The possible medium descriptions for the soil, vadose and aquifer zones are presented in Tables I-3 to I-5, respectively. Using the area measurements and the description of each sub-setting, area-weighted frequency histograms of depth to water, net recharge, and hydraulic conductivity were developed for each hydrogeologic setting and are presented in Figures I-1 through I-22. For each hydrogeologic setting, Figures I-1 through I-22 portray the area-weighted frequency with which the possible ranges of values for depth to water, net recharge, and hydraulic conductivity occur. Area-weighted frequency histograms for the descriptions of the soil, vadose zone, and aquifer media were also developed for each hydrogeologic setting and are presented in Figures I-1 through I-22 also.

Note that hydrogeologic settings that comprise less than 10 mile² were not considered in the analysis of Ross County performed in Chapter 3 . These include 7Ab, 7Ad, 7Ba, 7Bc, 7Be, 7F, 7Gb (Table I-1).

USE OF THE DRASTIC FREQUENCY HISTOGRAMS IN CHAPTER 3

From this information, frequency distributions for each hydrogeologic setting were roughly approximated for each of the input parameters required by SoilRisk as described below and summarized in Chapter 3, Tables 1 and 4. The soil-water volumetric flux rate (J_w , m/day) was assumed to be equal to the DRASTIC parameter recharge (m/day). The groundwater Darcy velocity (V_d , m/day) was derived from the relationship $V_d = K \cdot i$ where K (m/day) is the DRASTIC parameter hydraulic conductivity and i (-) is the hydraulic gradient, assumed equal to 0.01.

The histograms for the soil, vadose zone, and aquifer media descriptions were used to identify the most common medium by area in each of the three zones in each hydrogeologic setting. The most common media are summarized in Chapter 3, Table 4.

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- Frederick, C. L. (1991). Ground water Pollution Potential of Ross County, Ohio (Ground water Pollution Potential Report No. 24). Ohio Department of Natural Resources, Division of Water, Groundwater Resources Section, Columbus, OH.

Table I-1: Key to DRASTIC hydrogeologic setting symbols and number of sub-settings in each for Ross County, Ohio† (Frederick, 1991).

Sym- bol††	Hydrogeologic setting title	No. of sub- settings	Area (mile ²)
6Da	Alternating sandstone, limestone, and shale-thin soil	36	69
6Fa	River alluvium with overbank deposits	19	19
6L	Shale	14	11
6M	Sandstone	16	28
7Aa	Glacial till over bedded sedimentary rock	42	32
7Ab	Glacial till over outwash	4	2
7Ac	Glacial till over limestone	39	28
7Ad	Glacial till over sandstone	4	6
7Ae	Glacial till over shale	57	86
7Af	Sand and gravel interbedded in glacial till	26	54
7Ba	Outwash	18	8
7Bb	Outwash over bedded sedimentary rocks	32	14
7Bc	Outwash over limestone	25	9
7Be	Outwash over shale	25	5
7C	Moraine	48	26
7D	Buried Valley	267	199
7Ec	Alluvium over sedimentary rock	45	17
7Ed	Alluvium over glacial till	32	13
7F	Glacial lake deposits	23	8
7G	Thin till over bedded sedimentary rocks	11	21
7Gb	Thin till over limestone	3	1
7Gc	Thin till over shale	11	35

†Total area of Ross County is 690 mile². †† A 6 indicates the hydrogeologic setting is in groundwater region 6; and a 7, groundwater region 7.

Table I-1: Standard DRASTIC Ranges for depth to water, net recharge, and hydraulic conductivity (Aller et al., 1988).

Depth to water (m) ^[1]	Net Recharge (m/day) ^[1]	Hydraulic conductivity (m/day) ^[1]
Range	Range	Range
0-1.5	0-1.4x10 ⁻⁴	0.04-4
1.5-4.6	1.4x10 ⁻⁴ - 2.8x10 ⁻⁴	4-12
4.6-9.2	2.8x10 ⁻⁴ - 4.9x10 ⁻⁴	12-28
9.2-15	4.9x10 ⁻⁴ - 7.0x10 ⁻⁴	28-41
15-23	7.0x10 ⁻⁴ - 1.2x10 ⁻³ ^[3]	41-82
23-30		82-285 ^[4]
30-46 ^[2]		

Notes: 1. DRASTIC uses units of ft, in/yr, and gpd/ft² for depth to water, net recharge, and hydraulic conductivity, respectively. The ranges have been converted to the metric units shown for use in this work. 2. DRASTIC category is 30+; maximum of 46 assumed. 3. DRASTIC uses 7x10⁻⁴+; maximum assumed based on the maximum difference between precipitation and evapotranspiration (Baes and Sharp, 1983). 4. DRASTIC uses 82+; maximum assumed based on hydraulic conductivity ranges for the Glaciated and Non-Glaciated Central Groundwater Regions given in Back et al. (1988).

Table I-3: Soil medium key (Frederick, 1991).

Symbol	Description
ta	thin or absent
g	gravel
s	sand
p	peat
sc	shrinking and/or aggregated clay
sl	sandy loam
l	loam
sil	silty loam
cl	clay loam
m	muck
nsc	non-shrinking/non-aggregated clay

Table I-4: Vadose zone medium key (Frederick, 1991).

Symbol	Description
til	glacial till
sc	silt/clay
sh	shale
ls	limestone
ss	sandstone
bls	bedded limestone, sandstone, and shale
sgs	sand and gravel with significant silt and clay
mi	metamorphic/igneous
sg	sand and gravel
b	basalt
kl	karst limestone

Table I-5: Aquifer medium key (Frederick, 1991).

Symbol	Description
msh	massive shale
mi	metamorphic/igneous
wmi	weathered metamorphic/igneous
gt	glacial till
bsl	bedded sandstone, limestone, and shale sequences
ms	massive sandstone
ml	massive limestone
sg	sand and gravel
b	basalt
kl	karst limestone

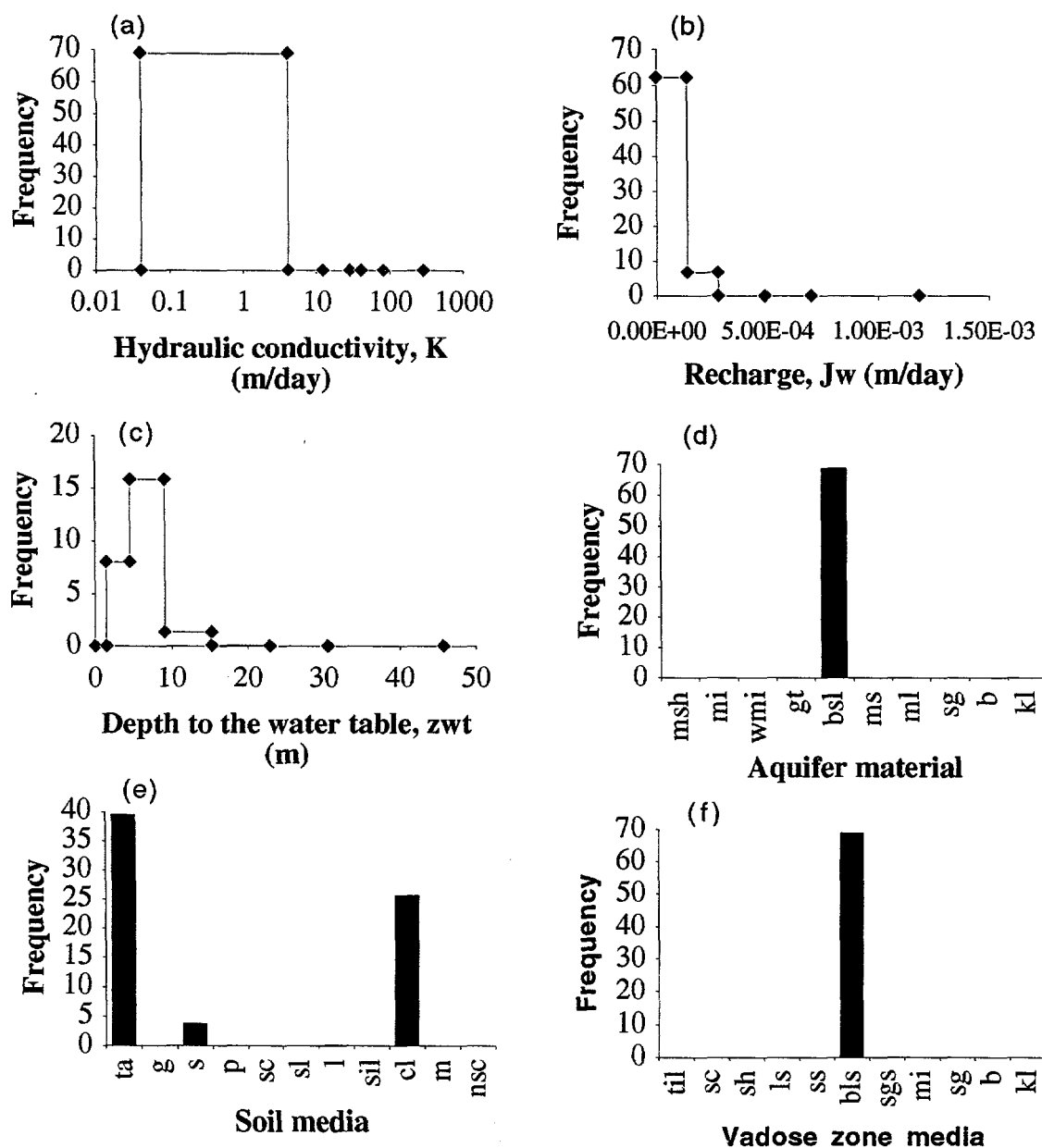


Figure I-1: 6Da Alternating Sandstone, Limestone, and Shale - Thin Soil
Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

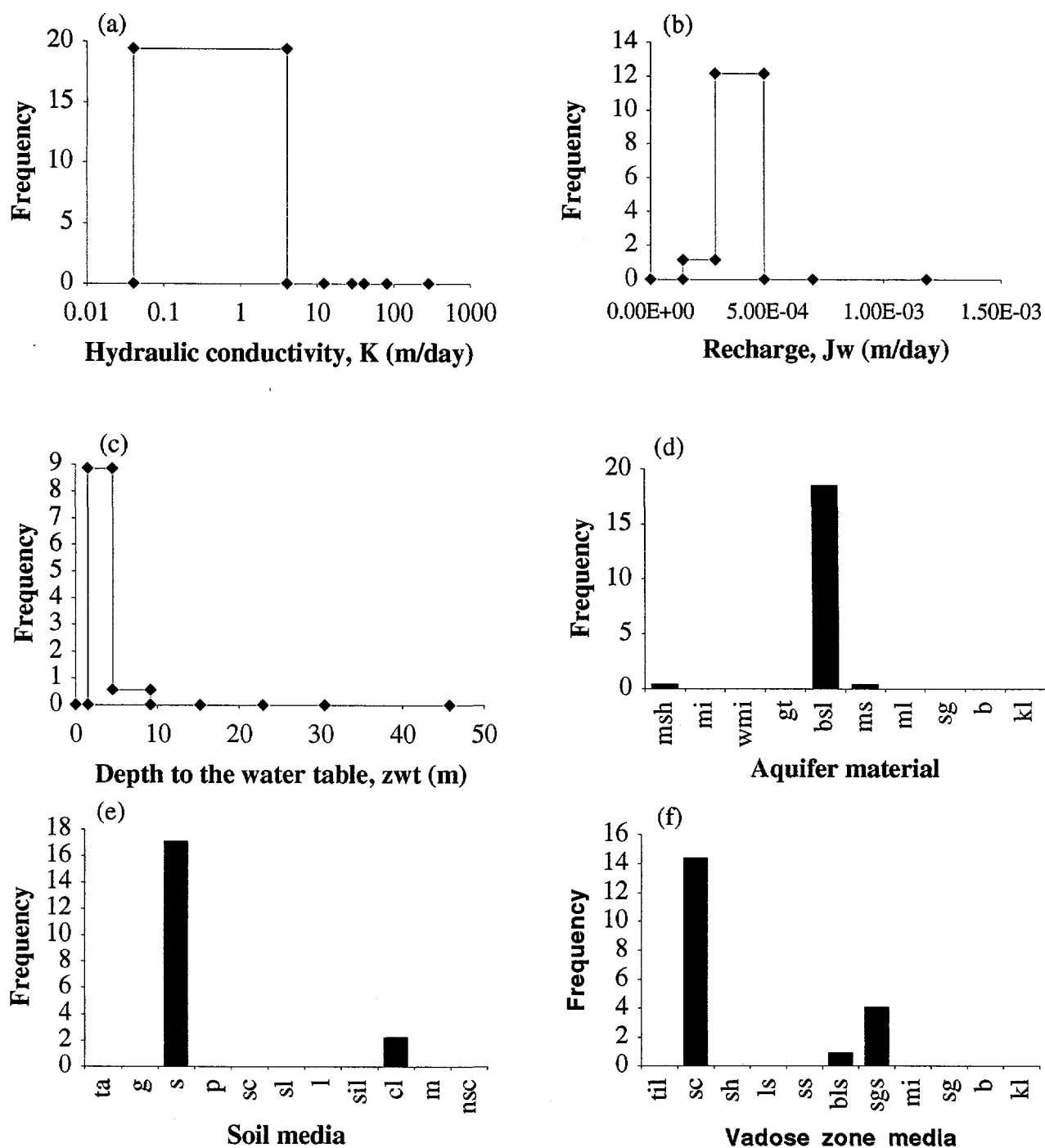


Figure I-2: 6Fa River Alluvium with Overbank Deposits

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

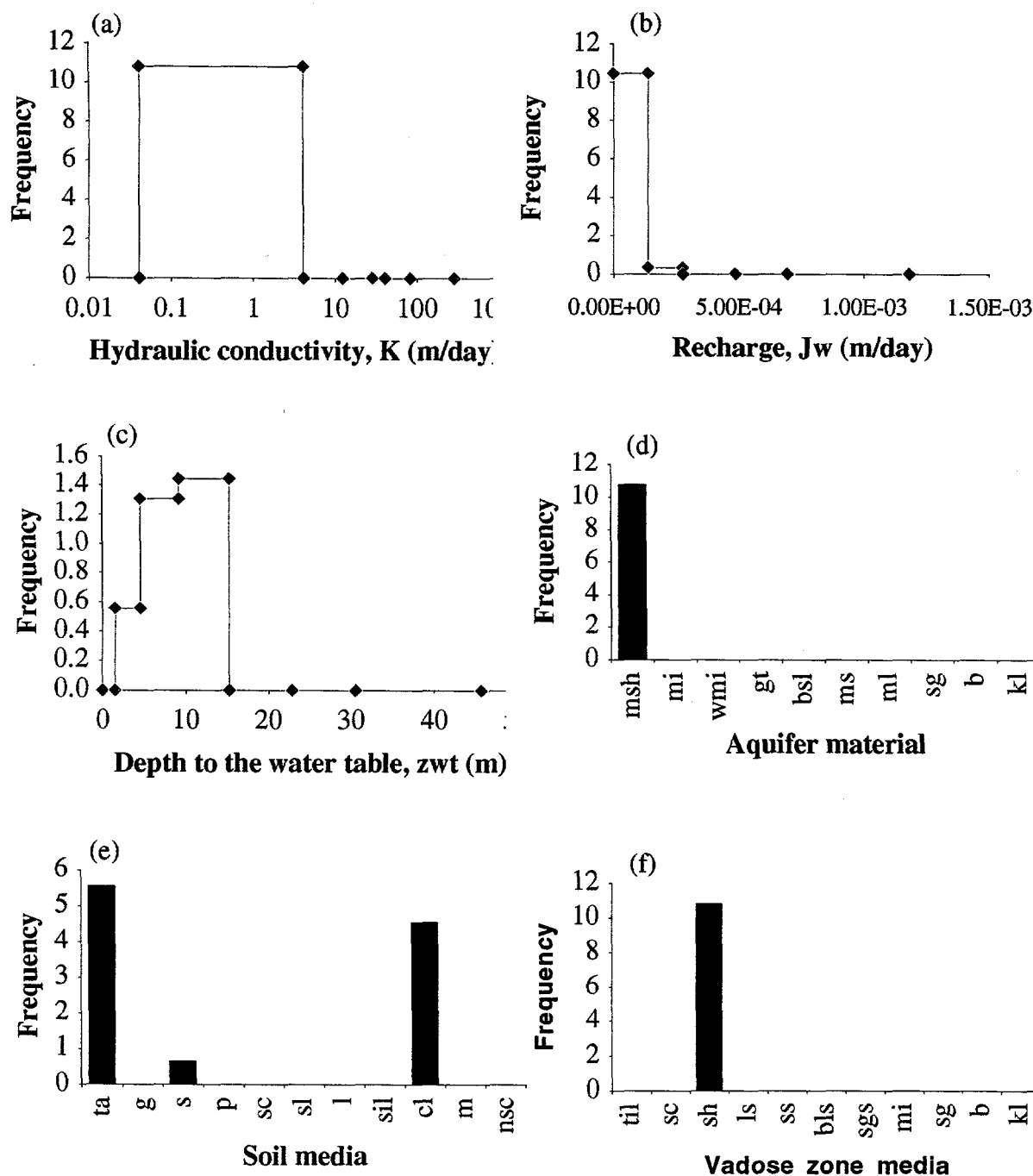


Figure I-3: 6L Shale

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

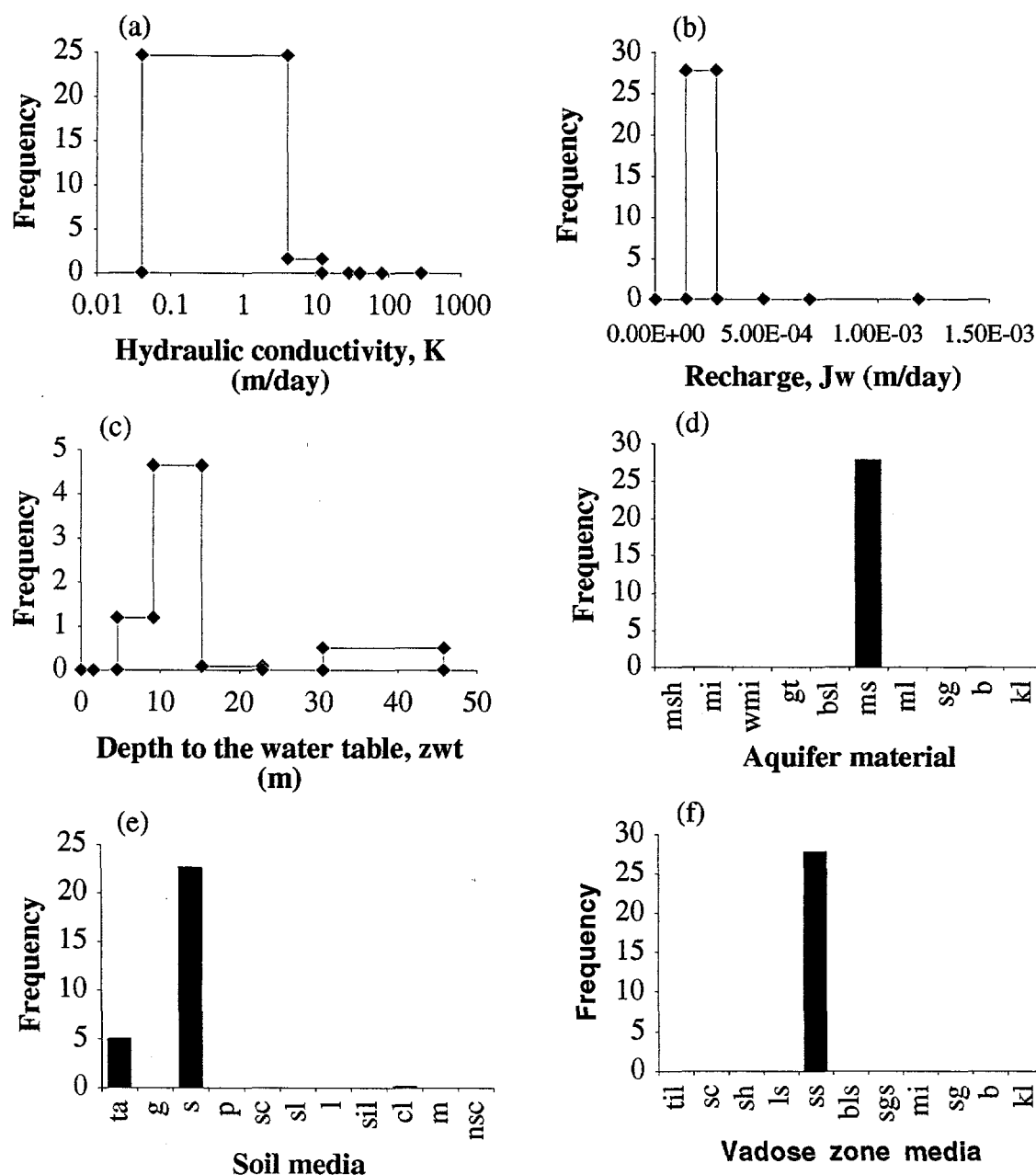


Figure I-4: 6M Sandstone
Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

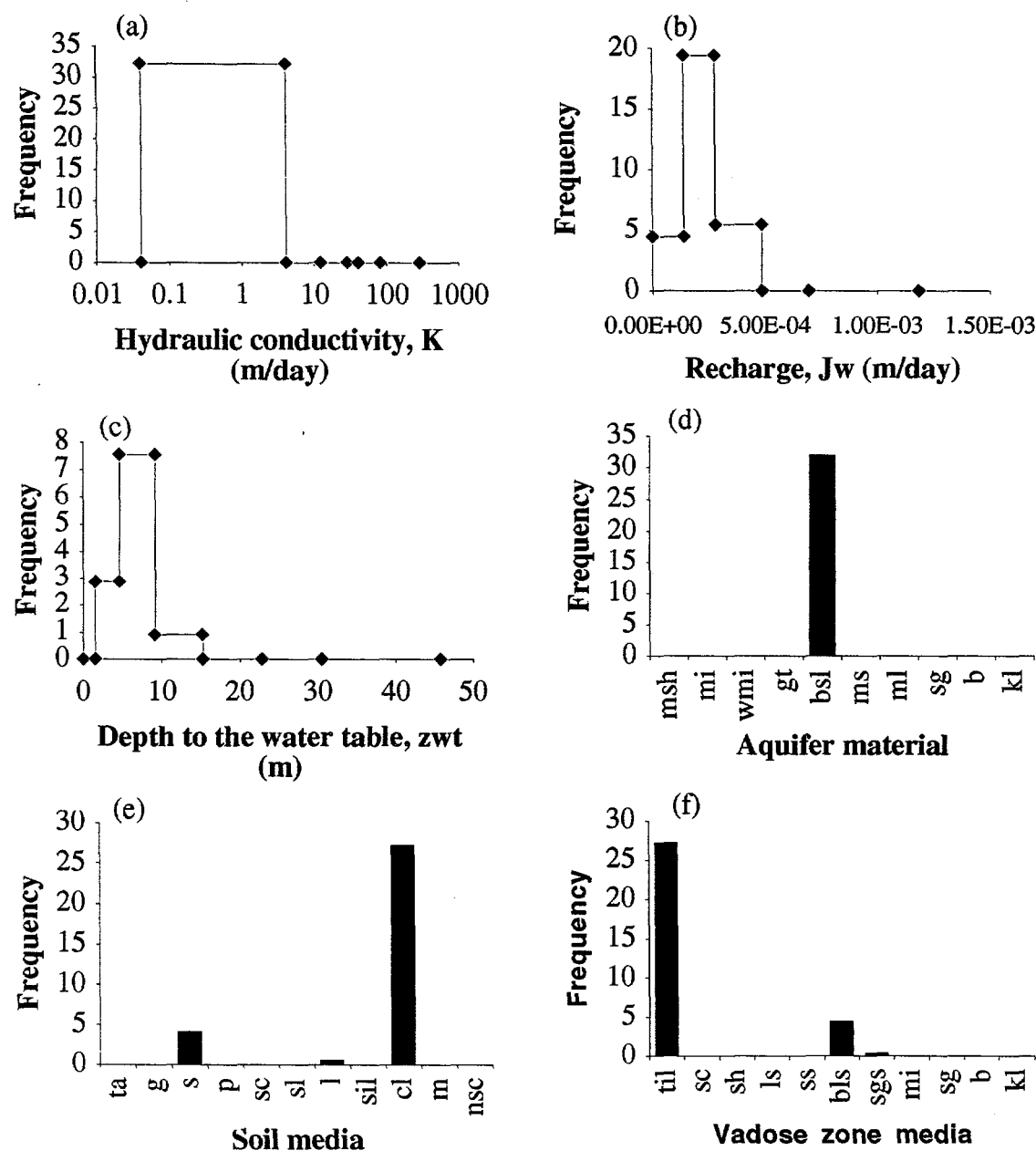


Figure I-5: 7Aa Glacial Till Over Bedded Sedimentary Rock
Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

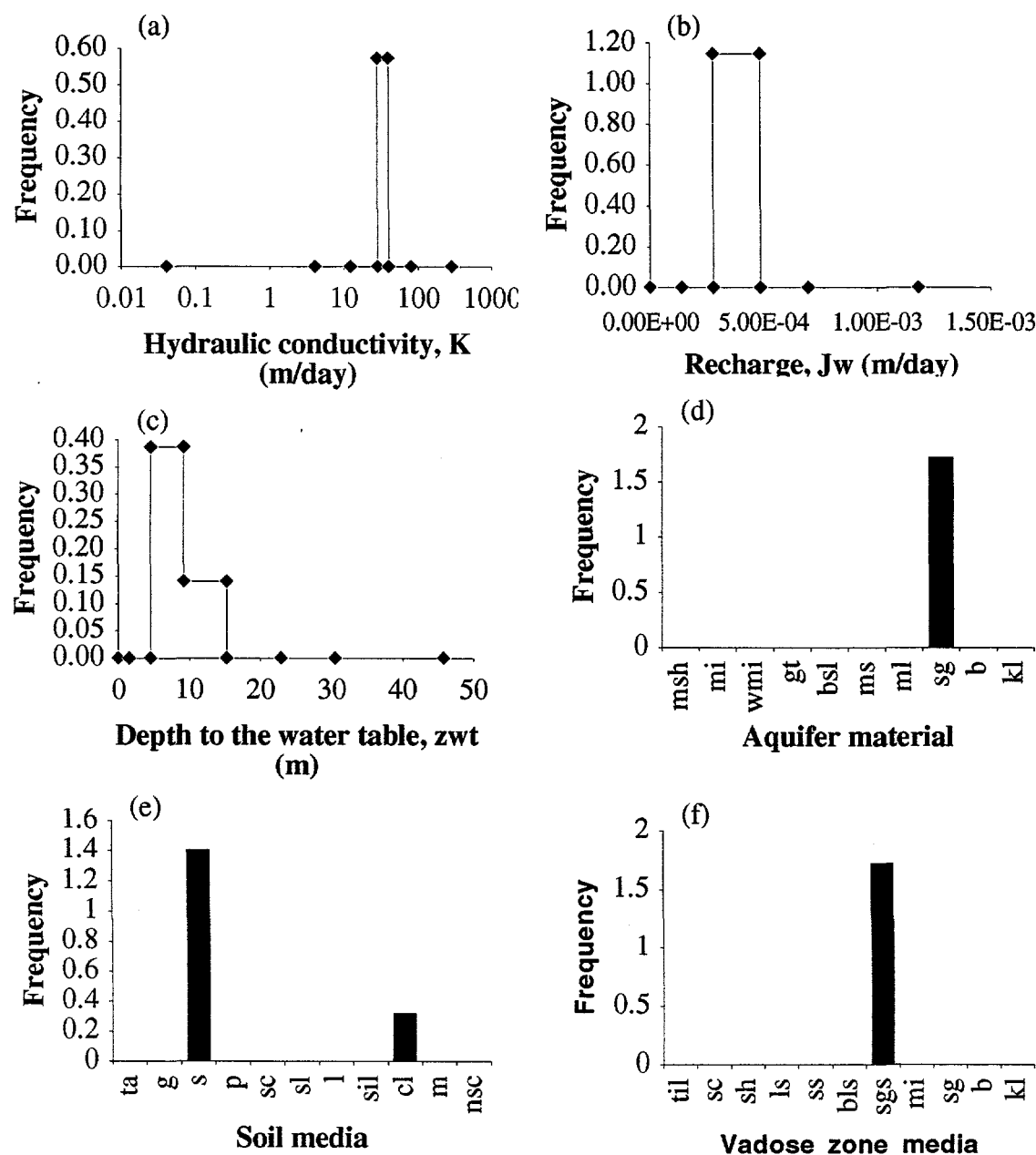


Figure I-6: 7Ab Glacial Till Over Outwash

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

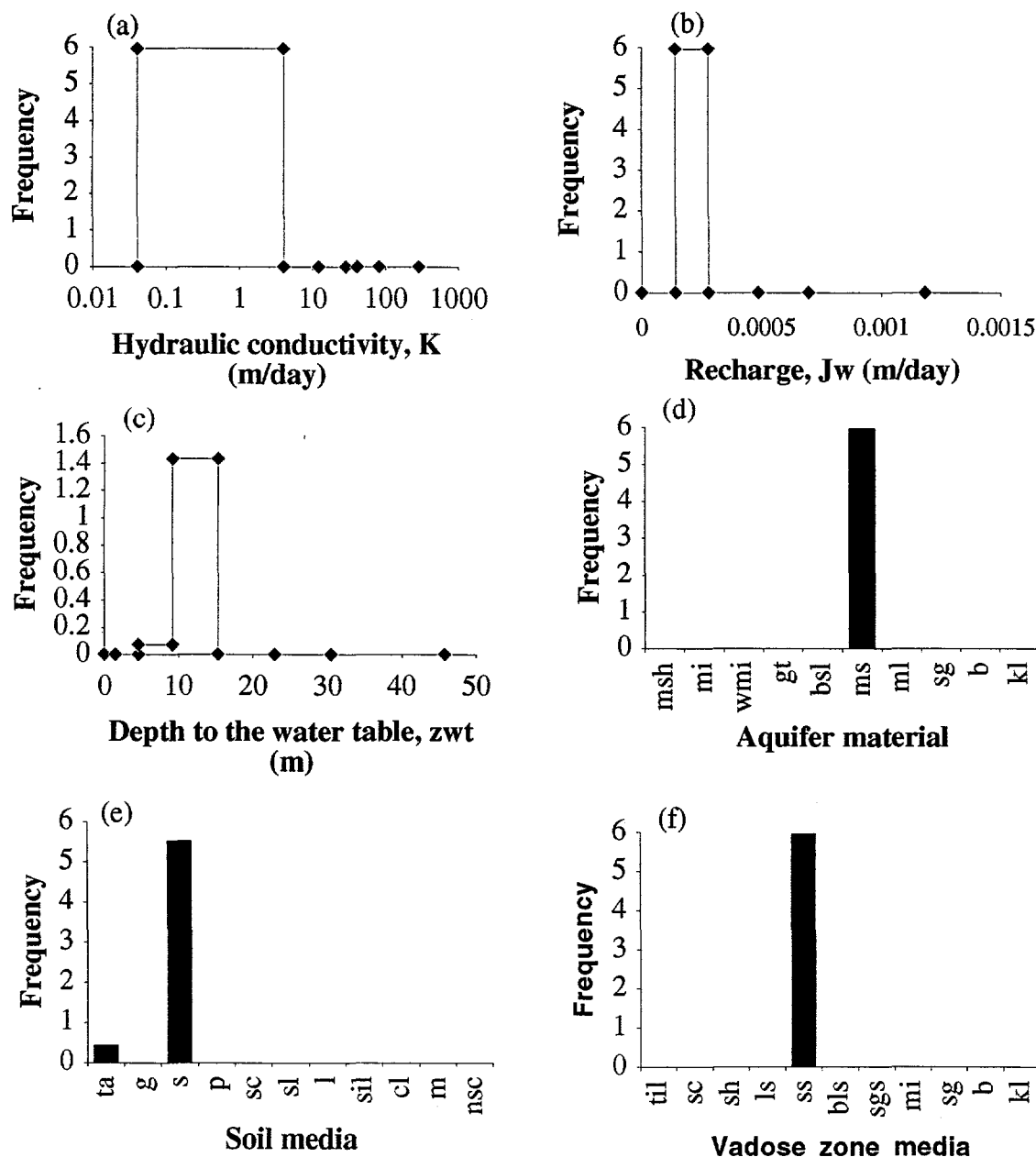


Figure I-8: 7Ad Glacial Till over Sandstone
Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

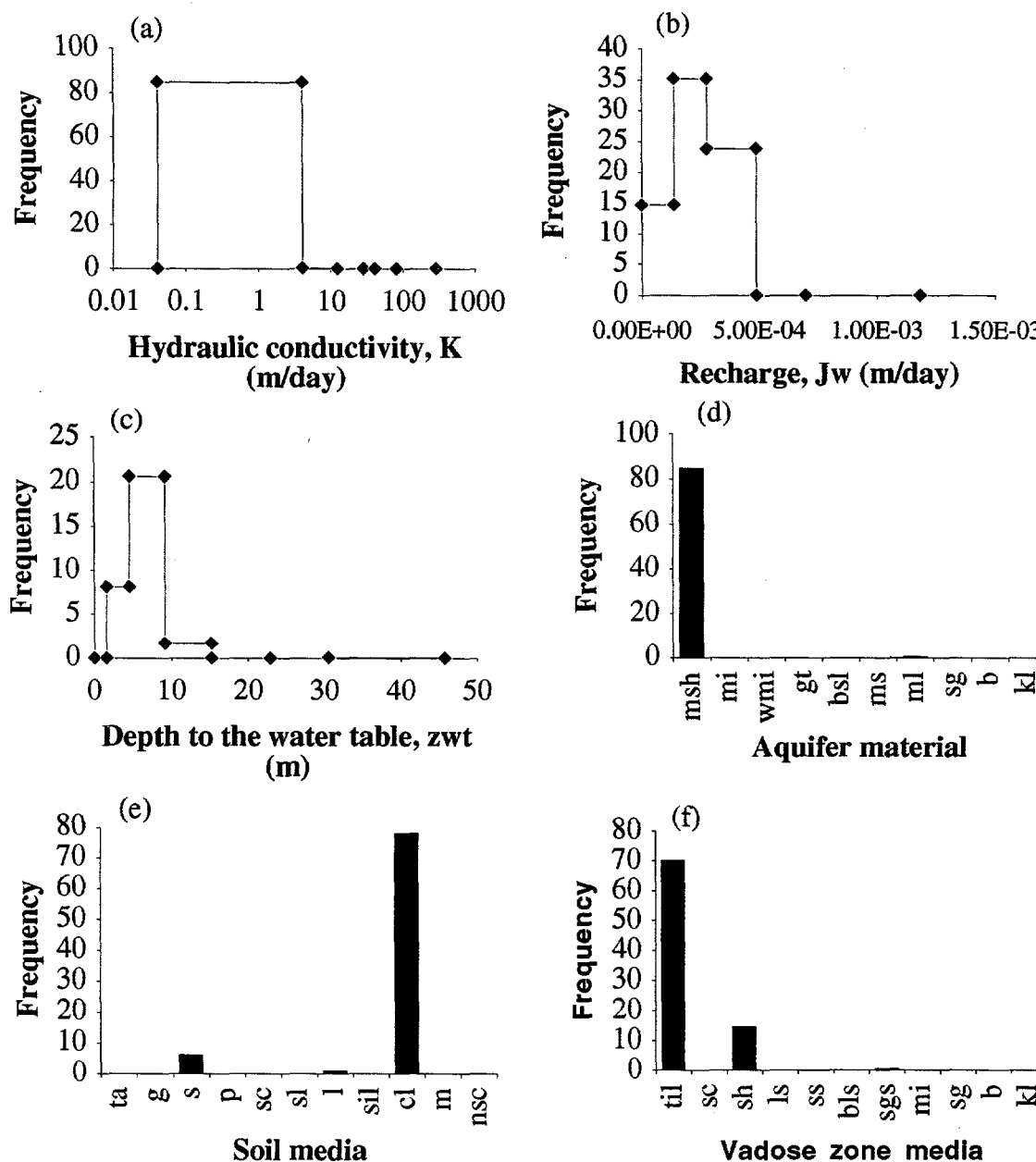


Figure I-9: 7Ae Glacial Till over Shale

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

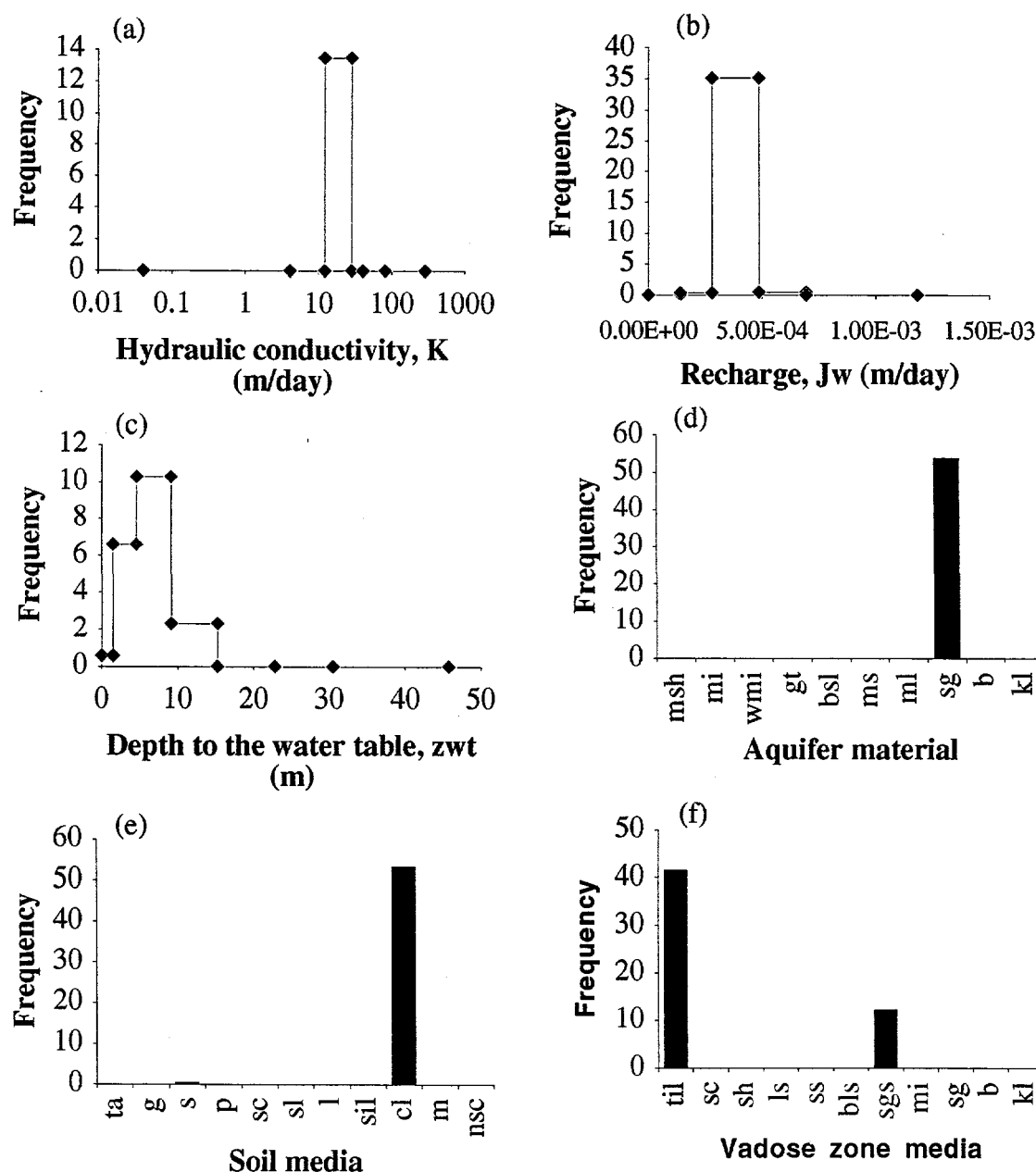


Figure I-10: 7Af Sand and Gravel Interbedded with Glacial Till
Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

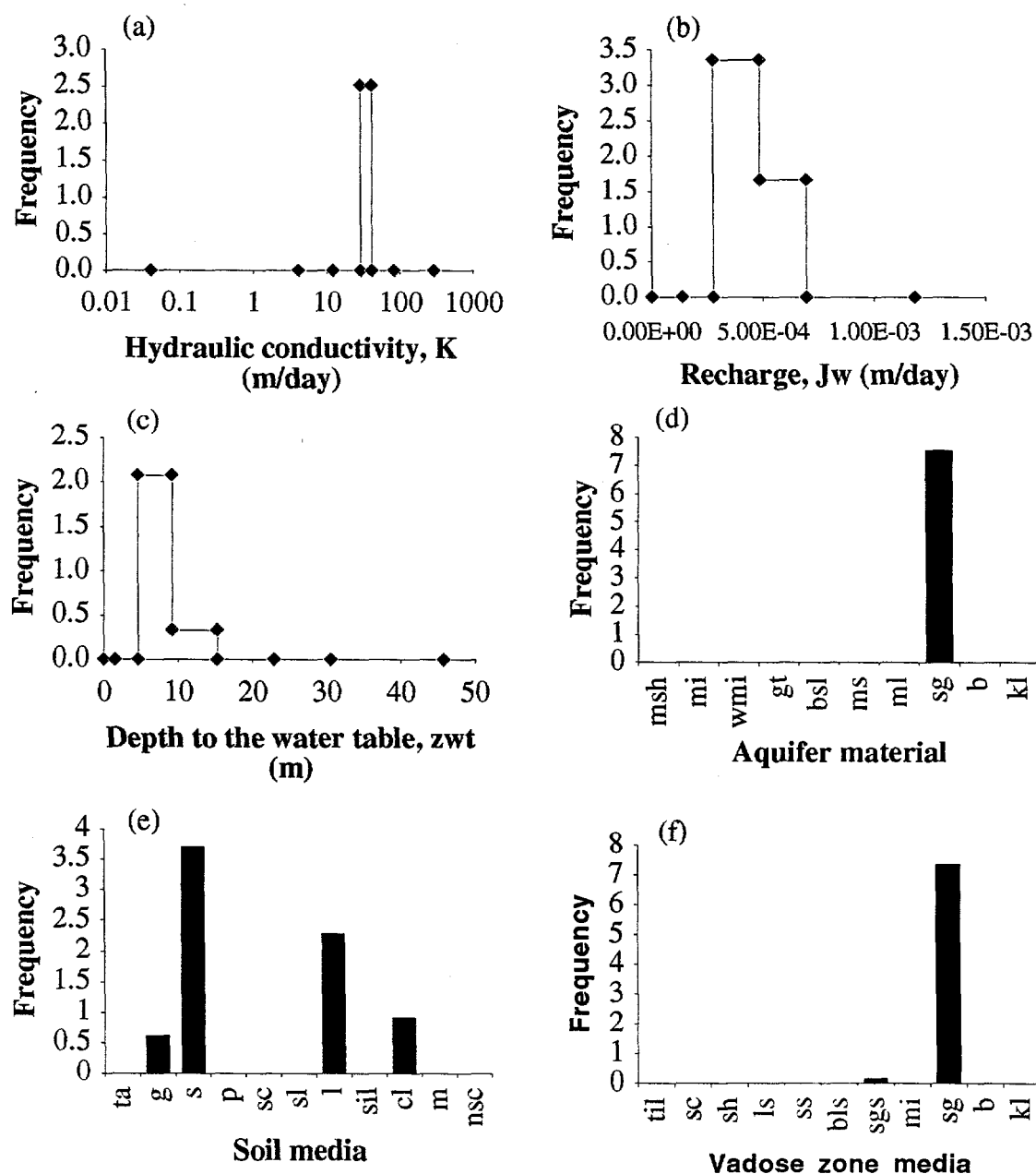


Figure I-11: 7Ba Outwash

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

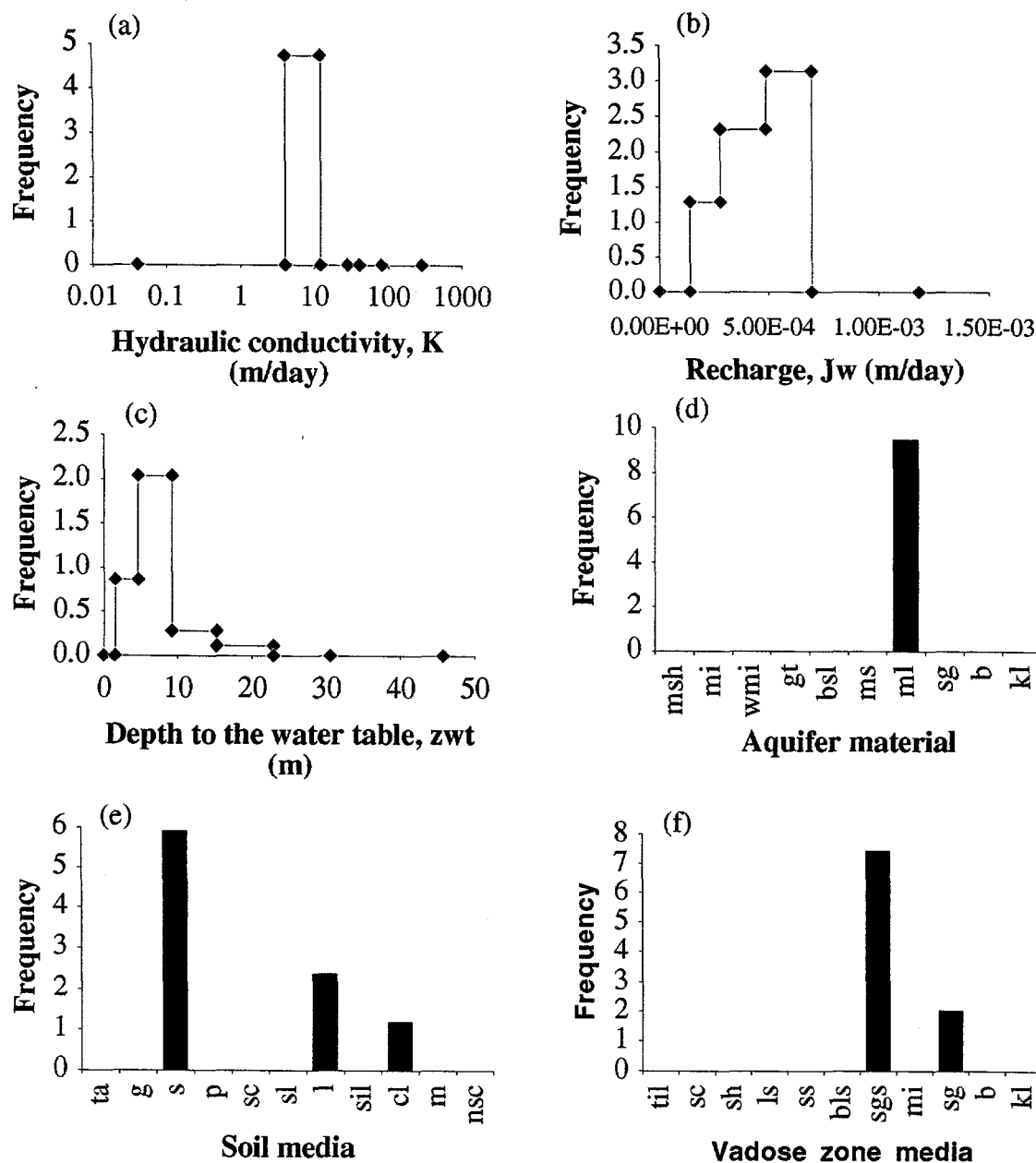


Figure I-13: 7Bc Outwash over Limestone

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

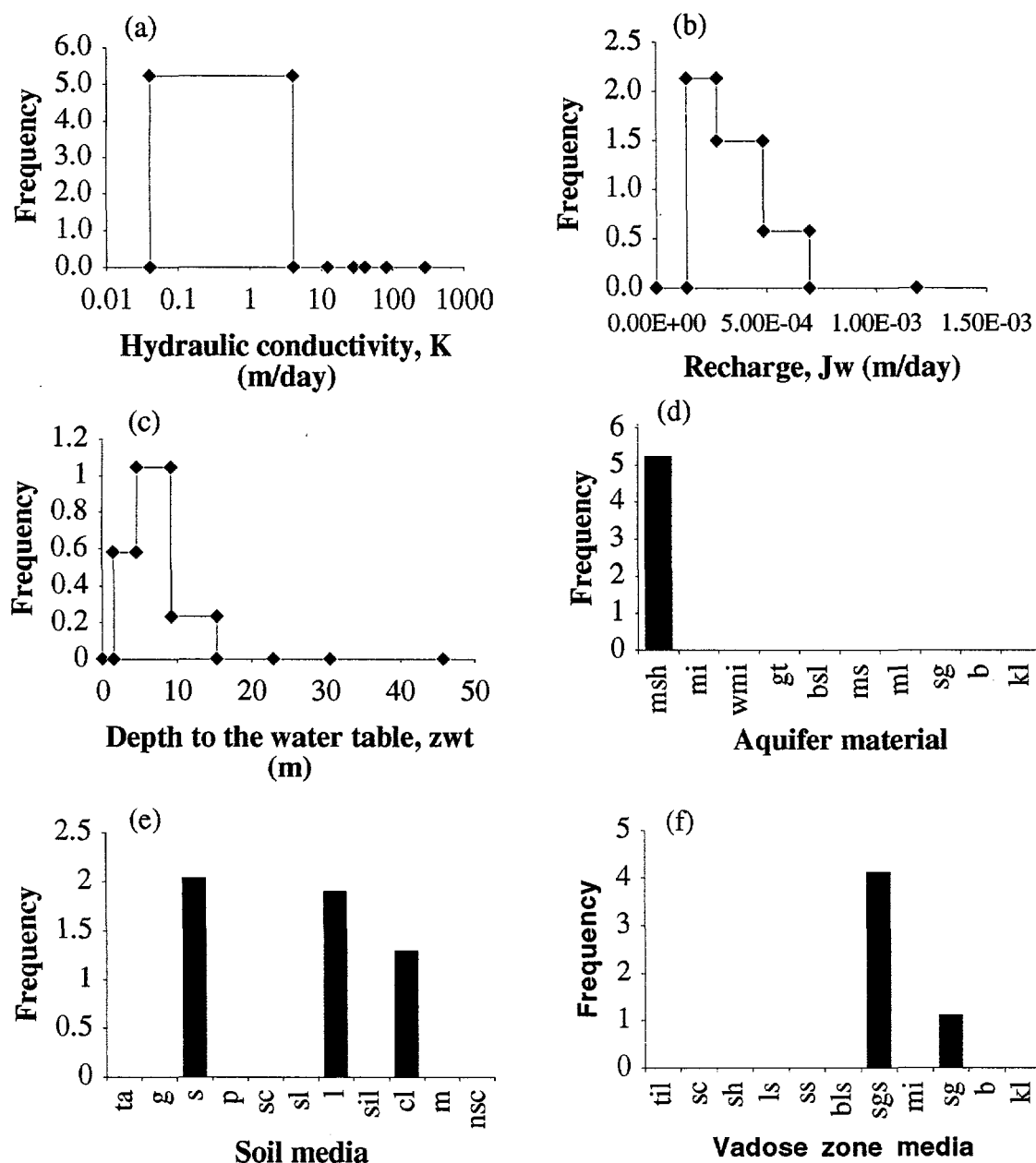


Figure I-14: 7Be Outwash over Shale

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

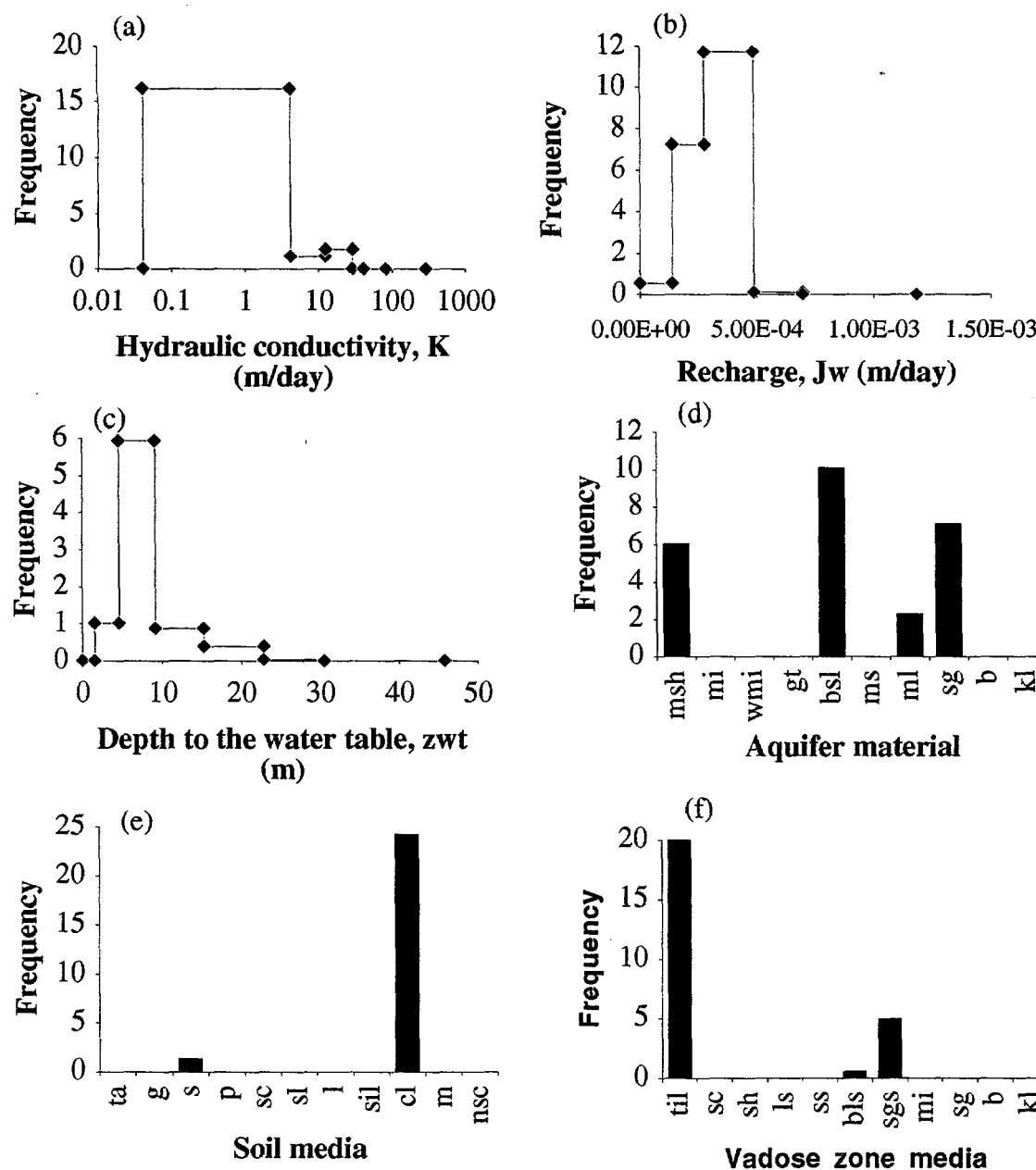


Figure I-15: 7C Moraine

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

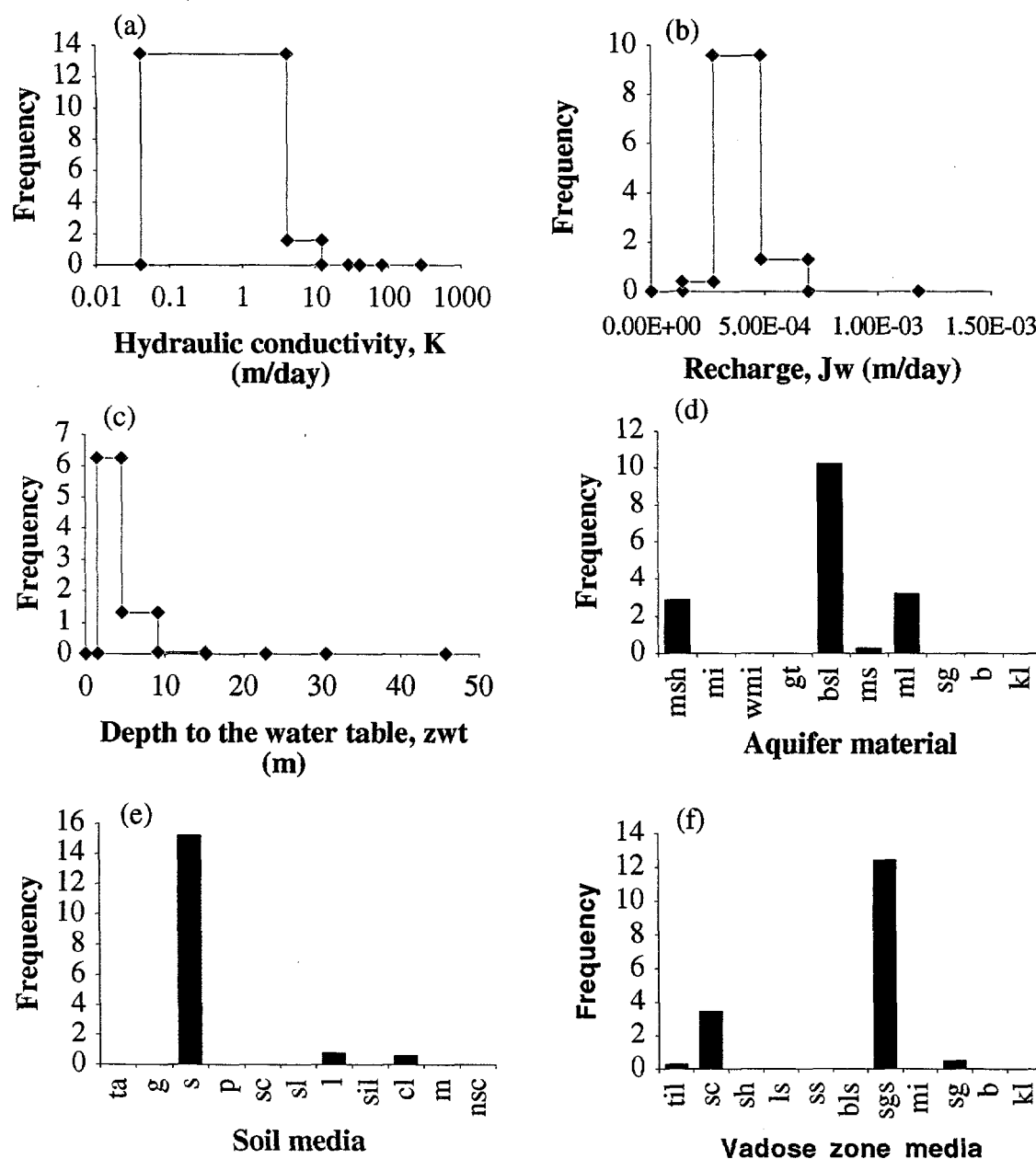


Figure I-17: 7Ec Alluvium over Sedimentary Rock

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

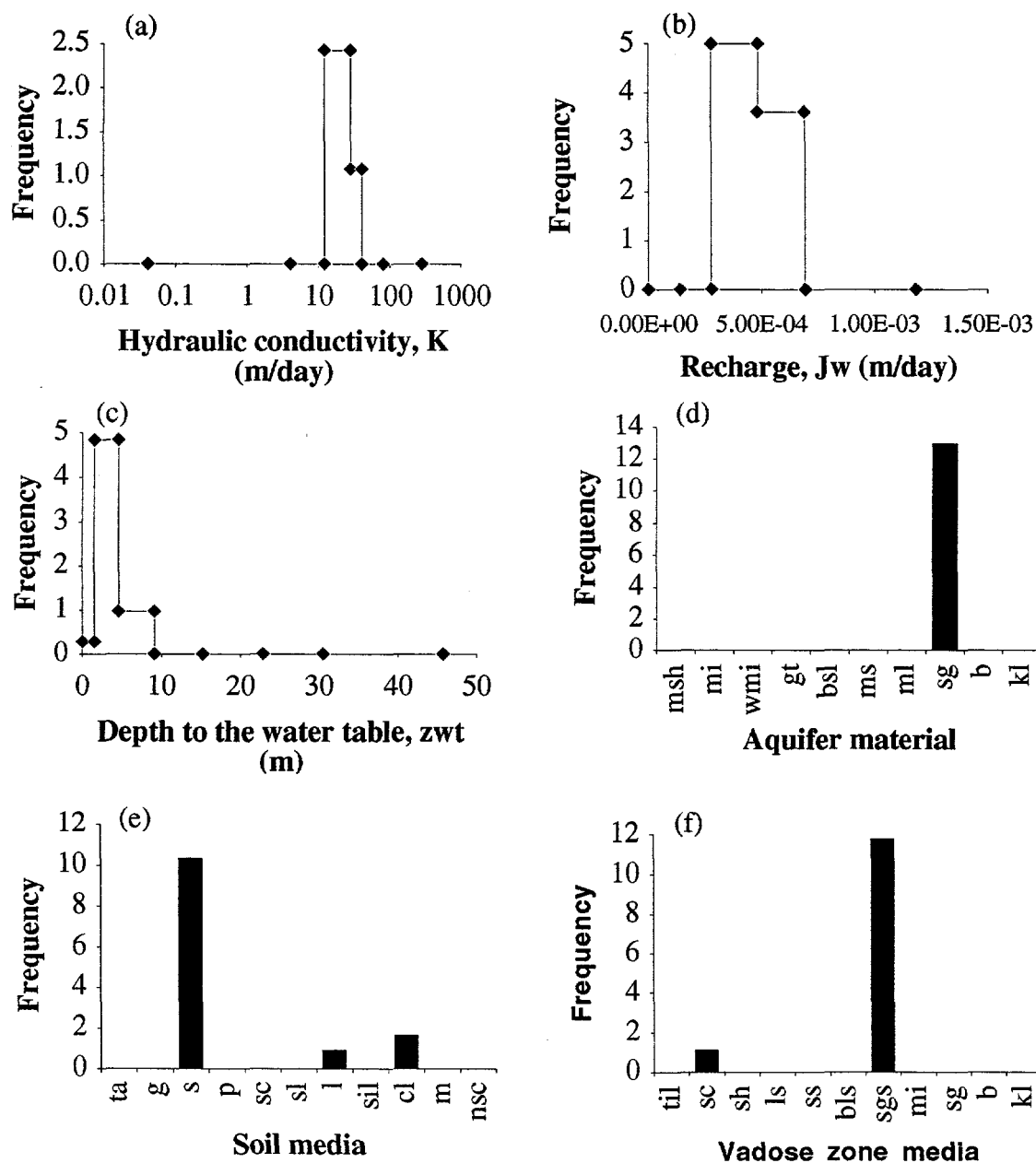


Figure I-18: 7Ed Alluvium over Glacial Till

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

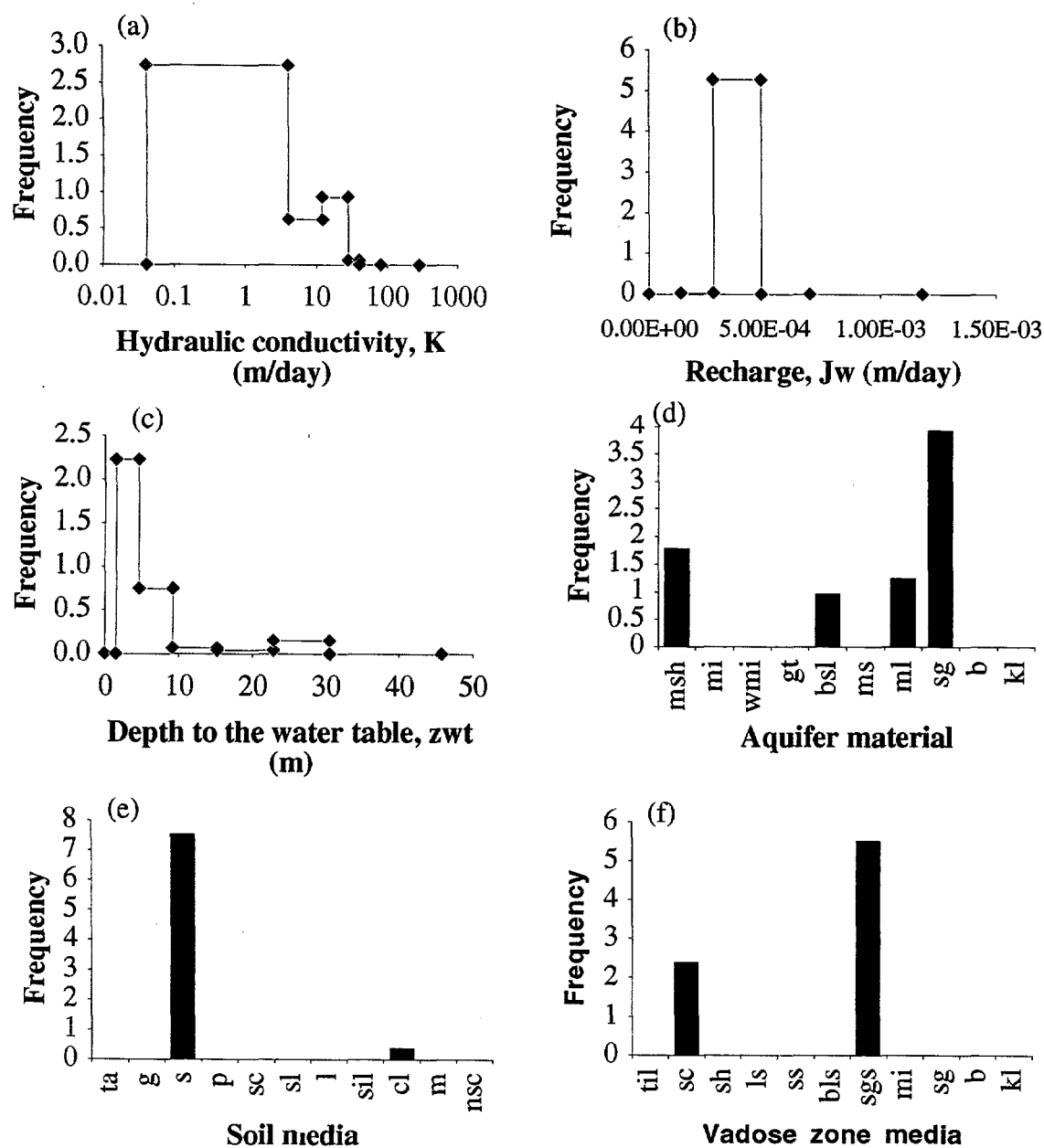


Figure I-19: 7F Glacial Lake Deposits

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

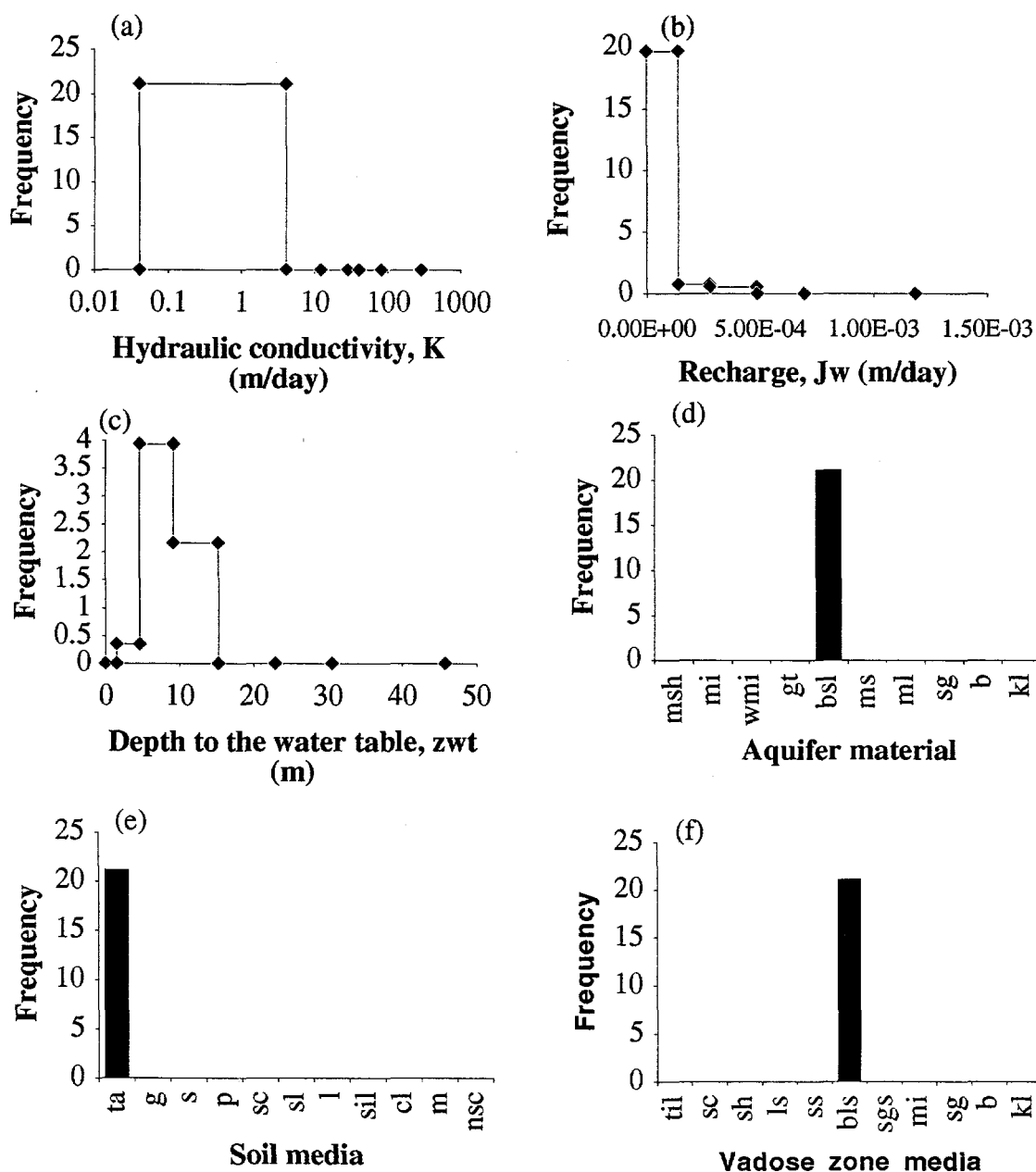


Figure I-20: 7G Thin Till Over Bedded Sedimentary Rock
Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

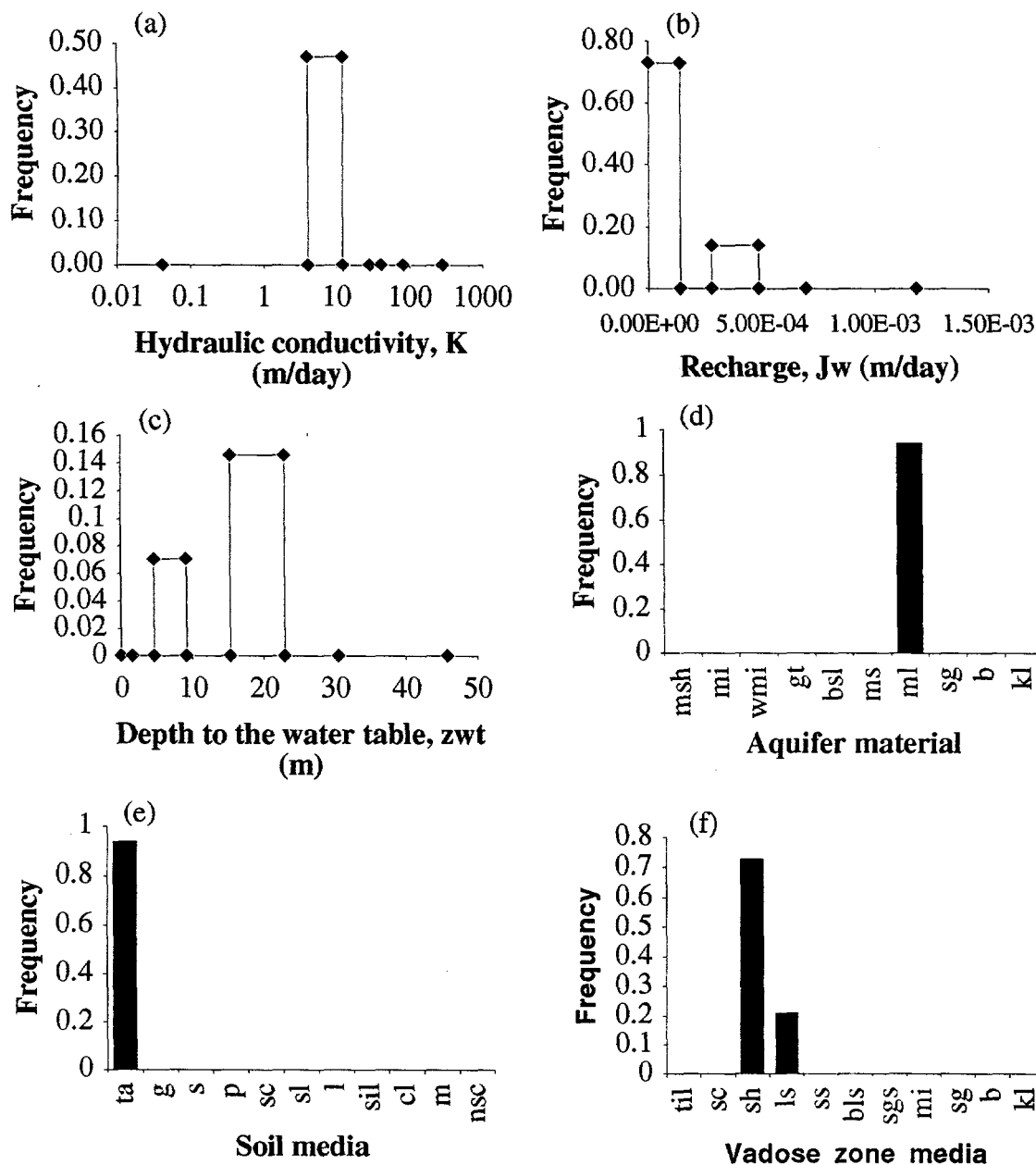


Figure I-21: 7Gb Thin Till Over Limestone

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

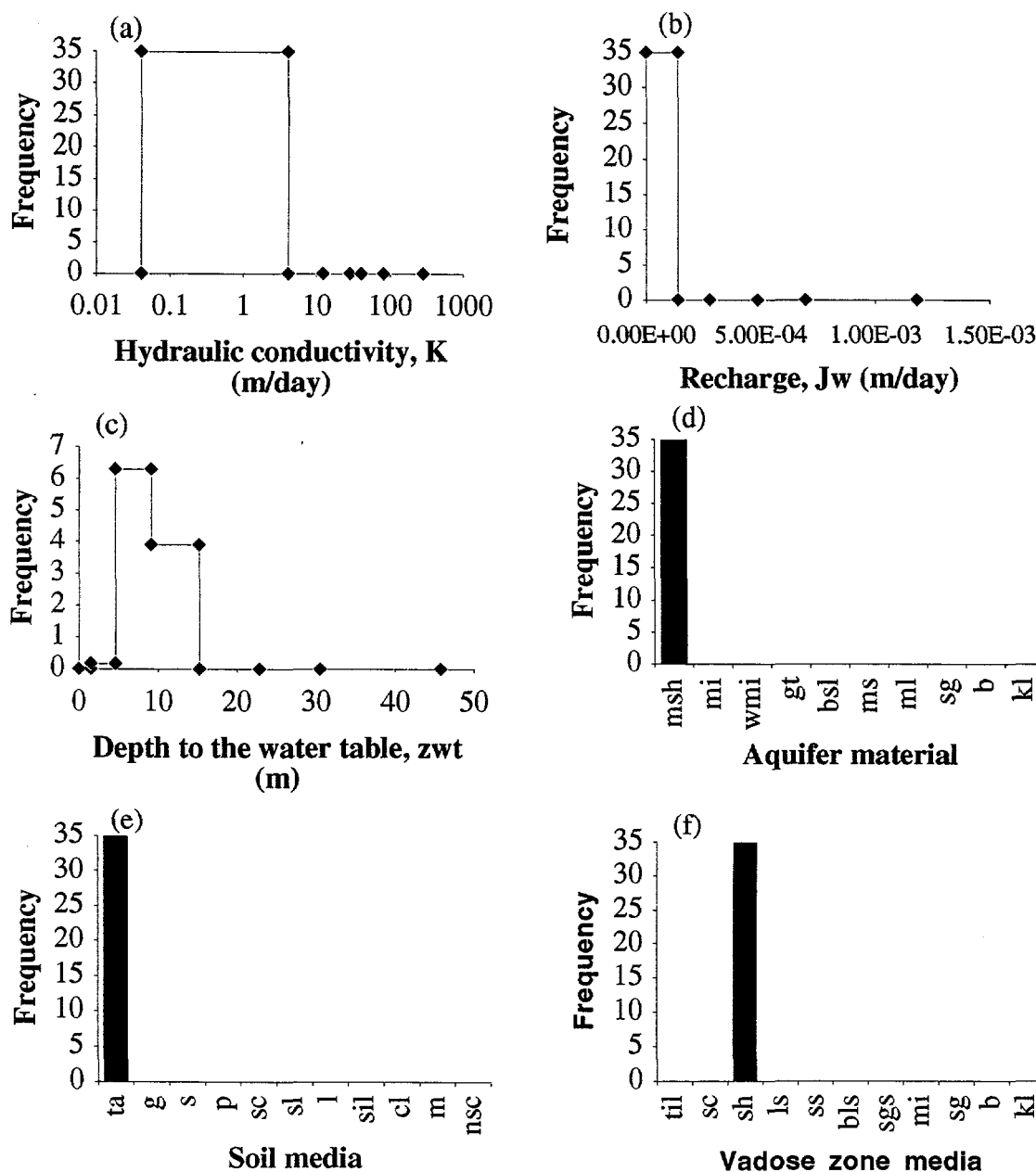


Figure I-22: 7Gc Thin Till over Shale

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

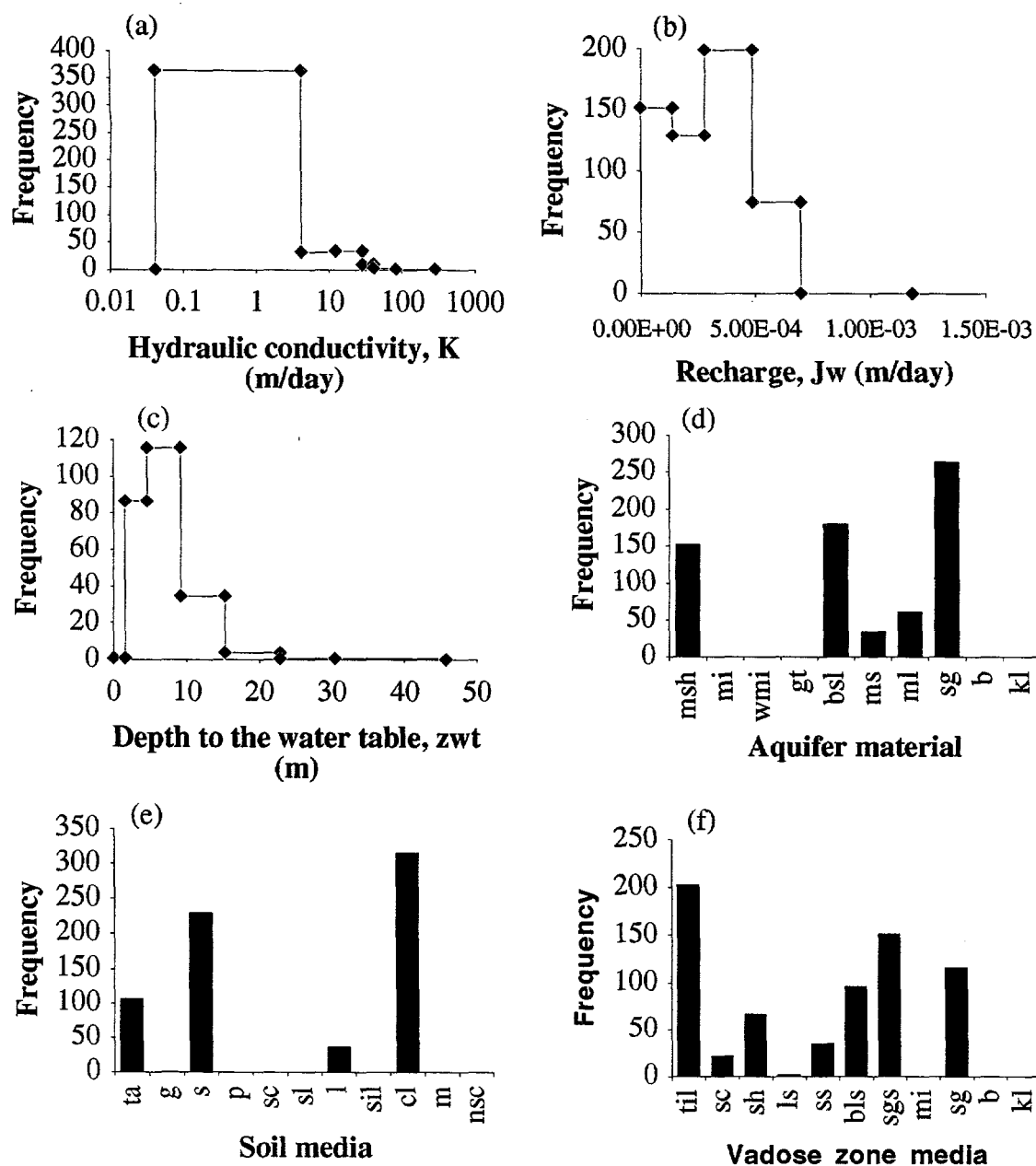


Figure I-23: Ross County

Area-weighted frequency histograms of the DRASTIC parameters (a) hydraulic conductivity, (b) net recharge, and (c) depth to water, and (d) aquifer, (e) soil, and (f) vadose zone media descriptions. See Tables I-3 to I-5 for a key to the aquifer, soil, and vadose zone media symbols.

APPENDIX J:
OVERVIEW AND CRITIQUE OF CURRENT UNIFORM
APPROACHES TO SETTING SOIL REMEDIATION GOALS

This appendix provides a brief overview of current approaches to setting uniform contaminant concentration levels in soil, and critiques the current approaches in light of the results of presented in Chapters 2 and 3. Interest in some form of a uniform approach is apparent by the number of agencies at the state and national level developing contaminant concentrations in soil to be used as remediation goals, screening levels, or guidelines at hazardous waste contaminated sites in their respective jurisdictions. States that have developed in final or draft form uniform soil remediation guidelines include Massachusetts (Campion et al., 1994), Pennsylvania (Pennsylvania Department of Environmental Resources, 1993), Wisconsin (Barden, 1994), and Tennessee (Tennessee Association of Business, 1991). New Jersey published proposed levels in 1992 (NJDEPE, 1992), but legislation was revised before they were finalized. The new legislation (SB#1070) also calls for uniform guidelines, but they have not yet been developed. (Interest at the international level is also apparent with uniform guidelines in place in several provinces in Canada, Great Britain, and the Netherlands (Ramsey et al., 1994; Siegrist, 1989). Uses of the uniform contaminant concentration levels developed range from clean up guidelines to screening levels above which site specific assessment is warranted. In addition, U.S. EPA Region III maintains and publishes regularly a list of contaminant concentrations in soil that are meant to be used as conservative guidelines, "relatively protective environmental concentrations at which EPA would not typically take action", in identifying environmental media of concern for baseline risk assessments (U.S. EPA, 1993b). U.S. EPA also has developed uniform draft soil screening levels to be used as "levels above which there is sufficient concern to warrant further study" (U.S. EPA, 1993a).

In most cases, the contaminant concentration levels for carcinogens were obtained by deterministic analysis of contaminant concentrations in soil to achieve a 10^{-6} risk goal assuming a residential exposure scenario with only one or two exposure routes and constant contaminant concentration in soil over the exposure duration (e.g., Pennsylvania

Department of Environmental Resources, 1993; U.S. EPA, 1993a; U.S. EPA, 1993b).

U.S. EPA Region III has developed alternative levels for the commercial/industrial exposure scenario and Massachusetts has developed alternative levels based on both level of exposure and groundwater classification.

When the groundwater pathway was considered, it was considered independent from other exposure routes. The soil guideline was set, not to meet a target risk level, but at a level at which the predicted *maximum* contaminant concentration in groundwater meets the Safe Drinking Water Act Maximum Contaminant Limit (MCL) in groundwater (e.g. U.S. EPA (1993a) and Wisconsin (Barden, 1994)). In predicting the contaminant concentration in groundwater as a function of contaminant concentration in the soil, EPA assumed a constant contaminant concentration in soil over the exposure duration, estimated the soil pore-water concentration using equilibrium partitioning, and applied a dilution attenuation factor to determine the concentration in groundwater.

The insights gained from the analyses performed in Labieniec et al. (1994a, b) are useful in critiquing the current approaches in the U.S. There is a common notion that it is conservative to assume constant contaminant concentration in the soil in developing uniform soil guidelines. While it may indeed be a conservative assumption, typically it does not yield a conservative result if potentially major exposure routes are ignored. For example, U.S. EPA Region III's guideline for benzene in soil is 22 mg/kg for a residential exposure scenario. It was calculated using a target risk of 10^{-6} , U.S. EPA default assumptions for the residential exposure scenario and a single exposure route, soil ingestion (U.S. EPA, 1991). Constant contaminant concentration in soil over the exposure duration was assumed. For comparison, the SoilRisk Model was used to calculate the total risk due to 22 mg/kg of benzene in soil using the median conditions at the representative site defined in Labieniec et al. (1994a) given an onsite residential exposure

scenario. Total risk was estimated to be 2×10^{-4} . This is two orders of magnitude higher than the 10^{-6} target risk used by EPA Region III. The discrepancy is marked considering the SoilRisk Model accounts for the loss of contaminant from the soil due to degradation, volatilization, and leaching. The reason for the large discrepancy is the fact that EPA Region III did not account for any exposure routes other than soil ingestion. The SoilRisk Model predicts that the major exposure route, given the conditions at the representative site, is the inhalation of soil gas infiltrating into an onsite residence. U.S. EPA used a similar approach to the one used by Region III to calculate the draft soil screening levels for surface soil, although they considered two additional exposure routes: vapor and dust inhalation.

With regard to the groundwater pathway, it should be noted that a different approach than that taken by U.S. EPA and others and described earlier was taken in the development of the SoilRisk model used in this work. It was developed so the *total* risk due to contaminated soil could be calculated as a function of the contaminant concentration in soil and exposure scenario. *Total* risk is the sum of risk due to all the exposure routes considered in any given exposure scenario. (See Labieniec et al. (1994c) for detailed descriptions of the exposure scenarios and routes considered.) The contaminant concentration in groundwater used in the exposure and risk equations was the *average* concentration over the exposure duration. This differs from an approach where the contaminant concentration in soil is set so that the maximum predicted concentration in groundwater meets the MCL.

This critique demonstrates the importance of modeling environmental fate and transport processes and considering all potentially major exposure routes in assessing total risk due to contaminated soil. It is also important to have an integrated total risk model when considering effect on the risk estimate of variable or uncertain site conditions because the

major exposure route is likely to differ for different site conditions. This was illustrated by the sensitivity analysis performed in Labieniec et al. (1994a).

It is also important to note the dramatic impact that the exposure scenario and assumptions associated with it have on the risk estimate. As mentioned earlier, four different exposure scenarios were considered in the analyses performed in Labieniec (1994a, b) and the median risk for the different exposure scenarios was found to differ by many orders of magnitude. This is illustrated in Figure 7 in Labieniec et al. (1994a) and Figures 4 and 7 in Labieniec et al. (1994b). It suggests that it would be useful to develop alternative uniform contaminant concentrations for different exposure scenarios as some of the states have already begun doing (e.g. Massachusetts).

An important issue not currently addressed by the current, mostly deterministic methods for calculating soil remediation goals is the specification of the target risk. When deterministic analyses is performed, contaminant concentrations in soil can be back-calculated to meet a deterministic target risk. When stochastic analyses are performed where the variability in site conditions are accounted for, the target risk must be specified along with a degree of confidence. For example, is the goal to achieve a 10^{-6} with 95% confidence, 80% confidence, or 50% confidence?

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