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Three Multimedia Models Used at Hazardous and Radioactive Waste Sites





THREE MULTIMEDIA MODELS USED AT HAZARDOUS AND RADIOACTIVE WASTE SITES

A Cooperative Effort by

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FOREWORD

This report was produced by the Interagency Environmental Pathway Modeling Working Group. The Working Group includes representatives of the U.S. Environmental Protection Agency - Offices of Radiation and Indoor Air, and Solid Waste and Emergency Response, the U.S. Department of Energy - Office of Environmental Restoration, and the U.S. Nuclear Regulatory Commission - Office of Nuclear Material Safety and Safeguards. The purpose of the Working Group is to promote the appropriate and consistent use of mathematical models in the remediation and restoration process at sites containing - or contaminated with - radioactive and/or mixed waste materials. This report provides an approach for evaluating and critically reviewing the capabilities of three specific multimedia models: MEPAS Version 3.0, MMSOILS Version 2.2, and PRESTO-EPA-CPG Version 2.0. These models are being used by the sponsoring Offices to support cleanup decision-making at various waste sites, and are of technical interest to them. The approach for model review advocated in this report is intended to assist technical staff responsible for identifying and implementing multimedia models in support of cleanup decisions at radioactive and hazardous waste sites. It is hoped that information in this report will enhance the understanding of these three models within the context of specific media components, human exposure and dose, and how they report uncertainty.

This document is one of several being developed by the Working Group to bring a uniform approach to solving environmental modeling problems common to all Federal agencies. The following are other reports prepared by this Interagency Working Group:

- Computer Models Used to Support Cleanup Decision-Making at Hazardous and Radioactive Waste Sites, EPA 402-R-93-005, March 1993.
- Environmental Characteristics of EPA, NRC, and DOE Sites Contaminated with Radioactive Substances, EPA 402-R-93-011, March 1993.
- Environmental Pathway Models Ground Water Modeling in Support of Remedial Decision-Making at Sites Contaminated with Radioactive Material, EPA 402-R-93-009, March 1993.
- A Technical Guide to Ground Water Model Selection at Sites Contaminated with Radioactive Substances, EPA 402-R-94-012, June 1994.
- Evaluating Technical Capabilities of Ground Water Models Used to Support the Cleanup of Low-Level Radioactive Waste Sites: A Critique of Three Representative Models, Draft, March 1994.
- Documenting Ground Water Modeling at Sites Contaminated with Radioactive Substances, EPA 540-R-96-003, January 1996.

The project Officers of the Interagency Working Group (Beverly Irla - EPA, Paul Beam - DOE, Sam Nalluswami - NRC) acknowledge the cooperation and insight of many staff in preparing this document from organizations including EPA/Environmental Research Laboratory, Athens Georgia: EPA Office of Radiation and Indoor Air Criteria and Standards Division, Washington, D.C.; and Batelle/Pacific Northwest Laboratories, Richland Washington. We would also like to thank all those from EPA Regions II, III, IV, V, VI, and VIII; EPA Office of Emergency and Remedial Response; EPA Office of Radiation Programs/Las Vegas; EPA National Air and Radiation Environmental Laboratory; DOE Office of Environmental Restoration, and NRC Office of Material Safety and Safeguards, who graciously agreed to provide review and comment. We also thank their managers who permitted them the time to provide us with valuable input.

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KEY ABBREVIATIONS USED IN THIS REPORT

- Ci Curie
- cm centimeter
- d day
- g gram
- kg kilogram
- km kilometer
- L liter
- m meter
- mg milligram
- min minute
- pCi pico-Curie
- s sec
- SI System Internationale
- Sv Sievert
- yr year

EXECUTIVE SUMMARY

Purpose

Multimedia models are used commonly in the initial phases of the remediation process where technical interest is focused on determining the relative importance of various exposure pathways. This report provides an approach for evaluating and critically reviewing the capabilities of multimedia models. This study focused on three specific models: MEPAS Version 3.0, MMSOILS Version 2.2, and PRESTO-EPA-CPG Version 2.0. These models evaluate the transport and fate of contaminants from source to receptor through more than a single pathway. They have been used to support cleanup decision-making at various sites and are of technical interest to the sponsoring organizations. The approach to model review advocated in this study is directed to technical staff responsible for identifying, selecting and applying multimedia models for use at sites containing radioactive and hazardous materials. The presence of radioactive and mixed wastes at a site poses special problems. Hence, in this report, restrictions associated with the selection and application of multimedia models for sites contaminated with radioactive and mixed wastes are highlighted. It is hoped that information in this report will enhance the understanding of these three models within the context of specific media components, human exposure and dose, and how they report uncertainty.

Report Structure

This report begins with a brief introduction to the concept of multimedia modeling, followed by an overview of the three models. The remaining chapters present more technical discussions of the issues associated with each compartment and their direct application to the specific models. In these analyses, the following components are discussed:

- Source Term
- Air Transport
- Ground Water Transport
- Overland Flow, Runoff, and Surface Water Transport
- Food Chain Modeling
- Exposure Assessment
- Dosimetry/Risk Assessment
- Uncertainty
- Default Parameters

The report concludes with a description of evolving updates to the model; these descriptions were provided by the model developers.

Model Selection

There are many multimedia models in use for simulating the transport, fate and effects of contaminants present at waste sites. All of these models could not be reviewed as part of this effort. Thus, the sponsoring agencies requested that MEPAS, MMSOILS, and PRESTO-EPA-CPG be reviewed because of their technical interest in these specific models. This should not be interpreted to mean that any of the agencies endorse any of these models or the specific findings presented in this report.

MEPAS, whose development was sponsored by the DOE, has a broad coverage of pathways and scenarios for radioactive and chemical hazardous materials. MMSOILS and PRESTO-EPA-CPG were developed by the EPA. MMSOILS is meant to be used for the screening and comparison of hazardous sites contaminated with toxic chemicals that are released from underground storage tanks, impoundments, waste piles, landfills, and injection wells. PRESTO-EPA-CPG was designed specifically to provide annual committed dose equivalent estimates from the release of radionuclides from low-level radioactive waste sites.

Model Components

Source Term

MEPAS is the most versatile of the three models, with the greatest ability to handle a variety of different types of source terms. Although the PRESTO-EPA-CPG model handles source terms only from near-surface trenches, its family of models can handle a variety of source terms, including contaminated soil, waste piles, deep-well injection, and underground tanks. MMSOILS is the only one of the three models reviewed here that performs a mass balance for the air and ground water pathways separately, relative to the initial source term. The generation of leachate into the ground water is estimated by different, but similar, means in all three models.

Atmospheric Pathway

A sector-averaged Gaussian plume algorithm is used by all three models to simulate the atmospheric transport of contaminants. The PRESTO-EPA-CPG model includes the effects of wet deposition and radioactive decay. The current version of the model does not include a volatile source term generation from a storage lagoon or lake. While the overall modeling capabilities of MMSOILS are similar to those of MEPAS, MMSOILS is less sophisticated in modeling the atmospheric pathway. It does not describe complex terrain, calms, depletion of the plume by wet deposition, and contaminant decay. MMSOILS cannot model releases from vents or stacks. However, this option is required only for modeling emissions from waste cleanup facilities, not from hazardous waste sites. The particulate emission models which are included in both MEPAS and MMSOILS are particles from wind erosion, vehicle traffic, and soil-

spreading operations. MMSOILS has a model of loading and unloading operations, but MEPAS does not. Finally, MEPAS has some capabilities which none of the other models have, namely, air sources (i.e., defining a source by ambient concentrations), calm meteorological conditions, and complex terrain.

Ground Water

Overall, MMSOILS has the most complex ground water pathway, since it alone uses a finite-element model for the unsaturated zone that incorporates layered heterogeneity. Unfortunately, there are two problems with simulating radioactive contaminants: (i) MMSOILS assumes that the contaminant does not decay while it is sorbed onto soil, and (ii) MMSOILS only models nonradioactive substances and does not explicitly simulate the ingrowth of progeny. Conceivably, the first problem could be overcome by entering a radioactive decay rate that is multiplied by the K_d . The second problem cannot be avoided easily, especially for short-lived contaminants. The PRESTO-EPA model employs a simple, one-dimensional model. MEPAS simulates ground water transport using a 3-D algorithm, but assumes that radioactive progeny have the same K_d as the parent. This can introduce error into the source and down-gradient concentration estimations.

Surface Water Transport

All three models take a rather similar, simplistic approach to modeling the surface water pathway. Both MEPAS and MMSOILS link ground water and surface water media by converting the ground water flux feeding into the surface water into an input flux to the surface water medium. The PRESTO-EPA-CPG model uses system equations representing the surface water, subsurface water, and atmospheric diffusion systems to calculate the rate of deep ground infiltration flow, overland flow, and the rate of evapotranspiration. If conditions allow, the overland flow may combine with the overflowing leachate. Then, this combined flow (with or without leachate overflow) interacts with the contaminated soil. The combined overland flow is programmed also to simulate the leaching of the contaminant out of the soil and transport into the nearby surface water to be pumped for human drinking, irrigation, and cattle feed. All three models employ the Universal Soil Loss Equation to estimate soil erosion across a site.

Food Chain Modeling

MEPAS includes food chains as an integral part of its exposure-dose component. Food chains are considered separately in MMSOILS and in PRESTO-EPA-CPG as agricultural data supporting exposure estimates. Although MEPAS can be used to model acute toxic atmospheric releases, all three models were designed primarily to handle long-term, chronic exposures. Each of the three models employ comparable, standard methods for estimating exposure to environmental contaminants through the food chain and other pathways. Therefore, the same limitations that exist for all exposure and risk assessments exist for these models. For example, food intake is subject to behavioral variations. Both the quantity and type of foods eaten vary from

Table S.1 cont'd. Summary of model features.				
	MEPAS	MMSOILS	PRESTO-EPA-CPG	
Bio-accumulation				
Animals	yes	ves	ves	
Terrestrial plants	yes	yes	yes	
Foliar deposition	yes	yes	ves	
Aquatic organisms	yes	yes	no	
Spatial definition	2-D	2-D	2-D	
Site Data Required	Extensive	Moderate	Moderate	
Contaminant Selection				
Hazardous chemical waste	yes	yes	no	
Radioactive waste	yes	no	ves	
Intakes from Ingestion of				
Drinking Water	yes	yes	yes	
Shower Water	yes	no	no	
Swimming Water	yes	yes	no	
Leafy Vegetables	yes ^{2 3}	yes	yes	
Other Produce	yes ^{2 3}	no	yes	
Meat	yes	yes	yes	
Milk	yes	yes	yes	
Finfish	yes	yes	yes	
Shellfish	yes	no	yes	
Special Food	yes	no	eggs	
Shoreline Sediment	yes	no	yes	
Soil	yes⁴	yes	yes	
Intakes from Inhalation				
While Showering	yes	no	no	
Of Air	yes	yes	yes	
Of Re-suspended Soil	yes	yes	yes ⁶	
Intakes from Contact				
While Showering	yes	no	no	
While Swimming	yes	no	no	
With Shoreline Sediment	yes	no	no	
With Soil	yes ⁴	yes	no	
With Volatiles in Air	yes	no	no	
External Exposures:				
While Swimming	yes	no	no	
While Boating	yes	no	no	
From Air	yes	no	ves	
With Soil	yes	no	yes	
With Shoreline Sediment	yes	no	no	
From Direct Radiation.	yes	no	no	

1 This component not available in 1993 version.

2. From air deposition on crops.

3. From irrigation of crops.

4. Estimations based on either measured concentrations or on calculated accumulations in soil after atmospheric deposition.

5. In the version modified for cleanup scenarios.

6. On-site scenario only.

7. MMSOILS only considers ground surface roughness in wind erosion of particulates.

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1. INTRODUCTION

Significant efforts are being made to remediate waste sites containing radioactive materials and hazardous wastes. The remediation goals may be based on reducing potential chemical or radiation doses to the public from all significant scenarios, media, and exposure pathways. Remediation strategies are typically based on an assessment founded on the use of computer models because of the complexities of sites and of the characteristics of the contaminants. These computer models use sets of mathematical equations incorporating many factors that cause or affect the movement of contaminants and radionuclides through various media including their intake by humans. Computer models are used now routinely by the U.S. Environmental Protection Agency (EPA) and others [e.g., Nuclear Regulatory Commission (NRC)] for setting standards and regulations, and by the U.S. Department of Energy (DOE) and others for determining the priorities and benefits of alternative cleanup options.

The EPA Office of Radiation and Indoor Air and Office of Solid Waste and Emergency Response, and the DOE Office of Environmental Restoration are attempting to develop a uniform approach to solving their common problems in environmental modeling for site remediation and restoration. As part of this effort, this report reviews in detail three multimedia models used by these agencies - MEPAS version 3.0, MMSOILS version 2.2, and PRESTO-EPA-CPG version 2.0.

The results of the analyses reported here are not intended as an endorsement of any of the models reviewed. Rather, the intention is to provide the reader with both an approach for evaluating mathematical models as well as an evaluation of each model's capabilities and limitations.

This report begins with a brief introduction to the concept of multimedia modeling, followed by an overview of the three models. The remaining chapters present more technical reviews of the sub-components of the models. Each chapter discusses first briefly the specific media component, then how each model handles radionuclide transport within that compartment, and finally describes evolving updates to the model.

In these analyses, the following pathway and risk assessment components are discussed:

- Source Term
- Air Transport
- Ground Water Transport
- Surface Water Transport
- Food Chain Modeling
- Exposure Assessment
- Dosimetry/Risk Assessment
- Uncertainty
- Default Parameters

The reviews are based on the following sources of information:

- Documentation from model developers, including Users' and Methods Manuals, Guides, Appendices, Revisions, and Addenda which explain or clarify the use or basis for each model.
- Reviews of models contained in the peer-reviewed literature and the results of formal review programs.
- Personal interviews with the models' developers to answer specific questions about features that are not discussed in the documentation, and to learn of proposed or expected developments for new versions of the models.
- Computer databases and expert systems, like the Integrated Model Evaluation System (USEPA, 1993b) and Exposure Models Library (USEPA, 1994a), that were developed to aid in selecting models appropriate for different applications.

The documentation available does not always describe upgrades or planned modifications because model building is an ongoing process. To this end, the developers of each model reviewed in this report were contacted and asked to provide a letter-report to update information contained in the model documentation. Improvements were summarized in the individual chapters.

2. MULTIMEDIA PATHWAY ANALYSIS

2.1 Media-Based Analyses

Multimedia modeling begins with a source of contamination and ends with a calculation of risk for the final assessment. Ideally, such a model would evaluate every possible pathway by which a contaminant is carried through every potential media from source to humans. Given a known or assumed concentration of a contaminant at a source and, from that, computing a risk is an extremely complex procedure. As stated by Seigneur et al. (1992):

"A comprehensive treatment of all these processes would require a multimedia transport model with fine spatial and temporal resolutions in all media, two-way inter-media transport, treatment of population dynamics with resolution of population cohorts according to activity patterns, age groups and physiological status; description of population exposure in a variety of micro-environments; and the development of accurate dose-response relationships."

Multimedia models may neither consider every potential pathway with the same thoroughness, nor every pathway between media. Even when some inter-media pathways are included, a model may not account accurately for the fate of material transported from one media to another. However, as Ryan (1993) pointed out, people may be exposed to contaminants indirectly through inter-media transport, as well as directly.

Several documents incorporating pathway analyses including estimating radiation dose in the environment were prepared for a variety of well-defined conditions. The Environmental Impact Statement (EIS) in support of licensing requirements for shallow land burial of low-level radioactive waste (10 CFR 61) is one example. Regulatory Guide 1.109 issued by the Nuclear Regulatory Commission is designed to be used for any release to the environment from effluent streams for any nuclear power plant. This document recommends how a generalized pathway analysis can be structured for a given effluent medium (air, water) in a particular environmental setting.

Figures 2.1 and 2.2 adapted from Dugan et al. (1990) illustrate simplified pathways for the release of radioactive and hazardous materials to the atmosphere and water, and their routes of exposure to humans. In these suggested transport models, air is contaminated by re-suspension and volatilization of radionuclides and chemicals. The roots of the plants take up the material. They are contaminated externally by the deposition of suspended particles. Herbivores take in radionuclides from the ingestion of soil, by grazing on contaminated vegetation, by drinking water, and by inhaling dust. The maximally exposed person is someone who lives in, and obtains their food from, the contaminated area, inhales contaminated air, drinks contaminated water, and ingests contaminated vegetation, meat, and dairy products from animals raised there.

People can be exposed to radioactive and hazardous contaminants present in the soil at National Priority List (NPL) and other sites through four basic environmental media: (i) the atmosphere: (ii) surface water, (iii) soil and ground water: and (iv) biota. The exposure pathways shown in Table 2.1 are considered by EPA to be typical of those to be included in any evaluation of human health conducted at a SUPERFUND site (Office of Emergency and Remedial Response, 1991).

Among these different media, a variety of inter-media transport mechanisms exist (Table 2.2). Choosing among the ones that should be included in any model requires balancing several competing concepts: modeling objectives, simplicity/complexity of the model; scenario/site complexity; data availability; and, the value of the information provided.

2.2 Level of Analysis

Practically, three levels of multimedia analysis can be identified (Whelan, et al., 1994):

- Screening-level (ranking)
- Analytical (prioritization and preliminary assessments)
- Numerical (detailed).

Early in the process, screening models are used to identify environmental concerns. These models are based often on a structured-value approach. They are designed to be used with regional/representative information. Models such as the EPA Hazard Ranking System (HRS) (USEPA, 1988b; USEPA, 1990b) divide the site and release characteristics into pre-determined categories that are assigned a point value based on answers to questions. The score from such systems is useful to determine if a situation is a problem, but not to provide a risk-based relative ranking of problems.

Detailed analyses require a highly specialized assessment of potential impacts. Methodologies such as the Chemical Migration Risk Assessment (CMRA) are composite-coupled approaches that use numerically based models that are not physically linked and represent single-medium models, implemented independently in series. This approach is reserved usually for the most complex models, is dataintensive, and relies on the expertise of the analyst. These detailed models are used to determine the levels of risk associated with relatively well-defined, complex problems, and tend to focus on special sets of problems and special types of situations. Although such tools are appropriate for their intended application, extension beyond site-specific applications is often either difficult or cost-prohibitive.

Analytical/Semi-Analytical/Empirical-Based multimedia models (designated as analytical models) can be used for prioritization or preliminary assessments. Most often, they are employed between initial screening and highly specialized numerical models. These models are the most versatile as they do not have the data constraints

of the numerical models, but are physics-based, unlike the structured-value models. The analytical models may contain some numerical computations (hence the semianalytical designation). The analytical models provide environmental evaluations through a wide range of applications. These models are fully coupled approaches that use analytically, numerically, and empirically based algorithms that are combined into a single code to describe each environmental medium.

Figure 2.3 illustrates the value of analytical models in the waste-site evaluation process. They can be used in a detailed (i.e., numerical) or an initial-screening (i.e., ranking/prioritization) assessment, where data and circumstances warrant. Figure 2.3 illustrates also the relative relationships between input-data guality, output uncertainty, and types of problems at each level of assessment. The computational requirements tend to be less at the earlier stages of an assessment when there are fewer available data and, correspondingly, the uncertainty with the output results tends to be greater. As assessment progresses, improved site-characterization the data and conceptualization of the problem increase, thereby reducing the overall uncertainty in risk estimates.

The analytical multimedia models integrate standard approaches into a consistent, yet powerful, tool. The multimedia models incorporate medium-specific, transport-pathway, and exposure-route codes that are based on standard, well-accepted algorithms. For example, these multimedia models employ analytical solutions to the advective-dispersive equations that describe transport in the ground water environment. When coupled, the models allow the analyst to immediately assess the entire process of contaminant release, transport, exposure, and risk at one sitting. Some models give the user the freedom to by-pass the transport components and use only the exposure/risk components. The value of a coupled model is exemplified by an order-of-magnitude reduction in assessment time, as compared to an uncoupled model.

Multimedia models assess concurrently multiple waste sites with multiple constituents to include baseline (at time = 0 yrs), no action (at time > 0 yrs), during-remediation, and residual (post-remediation) assessments, including changing land-use patterns (e.g., agricultural, residential, recreational, and industrial). The multimedia models can describe the environmental concentrations within each medium at locations surrounding the waste. Spatially distributed, three-dimensional, concentration isopleths can be constructed detailing the level of contamination within each environment. Three-dimensional risk isopleths can be developed by coupling land-use patterns with the environmental concentrations.



Figure 2.1 General air pathways to humans (after Dugan et al., 1990).



Figure 2.2 General liquid pathways to humans (after Dugan et al., 1990).

e 2.1. Typical e	xposure pathways by medium for residential a	ind commercial land uses.				
	Exposure Pathways, Assuming					
MEDIUM	RESIDENTIAL/RECREATIONAL LAND	COMMERCIAL/INDUSTRIAL LAND				
	USE	USE				
Ground Water	Ingestion from drinking	Ingestion from drinking				
	Inhalation of volatiles	Inhalation of volatiles				
	Dermal absorption from bathing	Dermal absorption				
	Immersion-external	Irrigation				
Surface Water	Ingestion from drinking	Ingestion from drinking				
	Inhalation of volatiles	Inhalation of volatiles				
	Ingestion during swimming	Irrigation				
	Ingestion of contaminated fish					
	Immersion - external					
Soil	Ingestion	Ingestion				
	Inhalation of volatiles & particles	Inhalation of volatiles & particles				
	Direct external exposure	Direct external exposure				
	Ingestion via plant uptake					
	Ingestion of meat, milk and other animal					
	products					
	Dermal absorption from gardening					

Tat	ble 2.2. Summary of major intermedia transport routes.
•	Transport from the Atmosphere to Land and Water
	Dry deposition of particulate and reactive gaseous pollutants
	Precipitation scavenging of gases and aerosols
	Adsorption onto particulate matter and subsequent dry and wet deposition
•	Transport from Water to Atmosphere, Sediments, and Organisms
	Volatilization
	Aerosol formation at the air/water interface
	Sorption by sediment and suspended solids
	Sedimentation and re-suspension of solids
	Uptake and release by biota
•	Transport from Soil to Water, Sediment, Atmosphere, or Biota
	Dissolution in rain water
	Adsorption on soil particles and transport by runoff or wind erosion
	Volatilization from soil and vegetation
	Leaching into ground water
	Re-suspension of contaminated soil particles by wind
	Uptake by microorganisms, plants and animals.



Figure 2.3. Relative relationships between input-data quality, output uncertainty, and types of problems addressed by each level of assessment (after Whelan et al., 1994.)

3. MODEL OVERVIEW

3.1 Introduction

A principal objective of modeling by the EPA, DOE. and NRC is to characterize the risks to human health presented by soil contamination present at sites containing radioactive materials, and the benefits to health derived from their cleanup. Estimates of the time-varying and time averaged radionuclide concentrations in air, surface water, ground water, soil and food items, intake of these materials by humans, and subsequent health risk are needed to fulfill this objective.

In the context of the exposure pathways identified in Chapter 2, the following end-points and processes are of particular importance:

- Individual and population doses and risks as a function of time
- External radiation exposures to radionuclides on the ground and in the air
- Radioactive decay and daughter ingrowth
- Indoor radon exposures

Through analysis of survey data (Moskowitz et al. 1993, Mills and Vogt, 1983, Case et al. 1989, USEPA 1989, USEPA 1990a), application of the EPA Integrated Model Evaluation System and the Environmental Models Library (USEPA 1993), review of scientific and vendor literature, and discussions with project staff, a list of models was identified that have been or could be used in a multimedia radiological risk assessment project. In developing this list, there was no attempt to determine initially whether these (Table 3.1) models could be appropriately applied to sites contaminated with radioactive substances.

Tables 3.2 and 3.3 give a brief description of representative ways in which each of the listed models has been used. The sponsoring Agencies requested that MEPAS, MMSOILS, and PRESTO-EPA-CPG be reviewed in greater detail. Each of these models was developed primarily for screening-type use or for comparisons between sites conducted for the purpose of ranking relative risk. These models were never intended for non-screening uses such as remedial design, etc. In addition to being designed primarily for screening, the three models are generic models; i.e., they are meant to be used at a wide variety of sites.

3.2 MEPAS

MEPAS (the Multimedia Environmental Pollutant Assessment System) is an analytical model designed by Pacific Northwest Laboratories, which was developed for, but is not limited to, use at CERCLA, Clean Air Act and Clean Water Act sites (Droppo et al., 1989, Volume 1). MEPAS is an enhancement of the Remedial Action Priority

System (RAPS, Whelan et al., 1987), using the same mathematical formulations and algorithms plus new additions to the methodology (Droppo, Whelan, et al., 1989). MEPAS was developed for DOE applications, but its development was specifically designed to address general problems at any hazardous waste site.

MEPAS develops an integrated, site-specific, multimedia environmental assessment. It can simulate the transport and distribution of contaminants (chemical and radiological) over time and space within air, water, soil, and food chain pathways. It estimates long-term health effects at receptor locations, from exposures over 70 years, as well as normalized maximum hourly concentrations for determining acute effects. Contaminated media and exposure pathways include air, ground water wells, water intakes from surface waters, recreation parks along surface water, on-site soil ingestion, and direct radiation. Receptors are evaluated as members of population and agriculture centers within an 80 km radius of the release unit. Currently, the model's database contains 576 referenced organic and inorganic chemicals and radionuclides. The database is updated and expanded continually. A "user-friendly" shell is provided with MEPAS which aids the user in defining the problem, entering input data, and executing the model run.

3.3 MMSOILS

MMSOILS (the Multimedia Contaminant Fate, Transport, and Exposure Model) was developed by the EPA Office of Research and Development as a "screening tool" for the "relative comparison" of hazardous waste (especially RCRA) sites (U.S. EPA, 1989a). It was designed specifically to simulate the release of toxic chemicals from underground storage tanks, surface impoundments, waste piles, and landfills. It can model the fate and transport of chemicals only, and calculates human exposure and health risk, as well as concentration in all important media. MMSOILS has a database for 240 chemicals. Like MEPAS, MMSOILS is provided with a "user-friendly" shell that aids the user in defining the problem, executing the model, and evaluating the output.

3.4 PRESTO-EPA-CPG

PRESTO-EPA-CPG (CPG for Critical Population Groups) belongs to a family of EPA exposure-assessment models which includes PRESTO-EPA-POP, PRESTO-EPA-DEEP, PRESTO-EPA-BRC, and PATHRAE-EPA (U.S. EPA, 1987). The PRESTO-EPA family of analytical models was designed specifically for radionuclide transport via natural processes, a consideration that dominates the overall structure and operation of their codes. PRESTO-EPA-POP (PRESTO for regional Populations) was the first in the series, and is the basis for each of the other models. PRESTO-EPA-CPG is designed to calculate the annual committed dose equivalent to members of a critical population group resulting from the disposal of low-level radioactive wastes (LLW) by a near-surface disposal method. The model identifies also the maximum effective dose equivalent and year of occurrence. POP models incidental, fatal, and genetic health effects to local and regional populations stemming from LLW deposited in shallow land burial sites also. This model can handle several different wasteforms within those

shallow-land disposal facilities: absorbing materials, activated metals, trash, solidified waste, and incinerated waste. It incorporates a database of 40 radionuclides. The PRESTO-EPA models are being modified currently to assess the health effects from a cleanup site by adding contamination scenarios not already included, namely: radon emission, soil and fish ingestion, and farming on site without protective cover.

Table 3.1. Some other representative multimedia models.						
MODEL NAME	PRIMARY REFERENCE	SPONSORING	HARDWARE			
		AGENCY	PLATFORM			
ARCL	Napier and Piepel, 1988	DOE	1			
DECHEM	Radiological Assessments	DOE	MSDOS-PC			
	Corporation	Ì				
DITTY	Napier et al., 1986	DOE				
DOSES	Oak Ridge National	ORNL				
	Laboratory					
DOSTOMAN	Root, 1981; King et al., 1985	DOE				
GENII	Napier et al., 1988	DOE/NRC	MSDOS-PC			
GEOTOX	McKone et al., 1983					
GWSCREEN	Root, 1991	DOE	MSDOS-PC			
HHEM	USEPA, 1991	EPA	Not yet			
			implemented			
HRS-1	Stenner et al., 1986	DOE	MSDOS-PC			
IMPACTS (PART 61)	Oztunali and Roles, 1986;	NRC	MSDOS-PC			
	Oztunali et al., 1986					
MEPAS	Doctor et al., 1990a,b,c;	DOE	MSDOS-PC			
	Droppo et al., 1989; Whelan					
	et al., 1987					
MILDOS	Strenge and Bander, 1981					
MILDOS-AREA	Yuan et al., 1989	DOE	MSDOS-PC			
MMSOILS	USEPA, 1992	EPA	MSDOS-PC			
MULTMED	Salhorta et al., 1990	EPA	MSDOS-PC			
NUREG 5512	Kennedy and Strenge, 1992	NRC	Not yet			
			Available			
NUTRAN	ROSS ET al., 1980	Atomic Energy	IBM Main			
ONICITE /MAAVIA	Nanior of al. 1004 Konnedy		Frame MCDOC DC			
et al. 1986: Kennedy, et al		NKC	MSDUS-PC			
	1 1 9 2 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2					
DATH1	Helton and Kaestner 1981		·			
	Campbell et al 1981	INC				
PATHRAE (-EPA)	Rogers and Hung 1987a	FPA	MSDOS-PC			
PC GEMS	General Sciences	FPA	MSDOS-PC			
	Corporation 1982		110000110			
PRESTO-EPA	USEPA 1983	EPA				
PRESTO-EPA-BRC	Rogers and Hung, 1987b	EPA				
PRESTO-EPA-CPG	Rogers and Hung, 1987d	EPA	MSDOS-PC			
PRESTO-EPA-POP	Fields et al., 1987a, 1987b	EPA	MSDOS-PC			
PRESTO-EPA-DEEP	Rogers and Hung, 1987c	EPA	MSDOS-PC			
PRESTO-II	Fields et al., 1986	<u>+</u>				
RESRAD	Gilbert, 1988	DOE	MSDOS-PC			
RISKPRO	General Sciences Corp. 1992	EPA	MSDOS-PC			
SARAH2	Vandergrift and Ambrose	EPA	MSDOS-PC			
	1988]				
UDAD	Momeni et al., 1979	NRC	<u> </u>			
UTM-TOX	Browman et al., 1982	1	+			

Table 3.2 - Examples of	of usage of other models.
MODEL NAME	DESCRIPTION OF REPRESENTATIVE USAGE
ARCL	Evaluate decommissioning alternatives by using a site-specific
4	radiation scenario/exposure pathway analysis to determine the
	acceptable levels of residual radioactive contaminants that remain.
DECHEM	Determine acceptable levels of chemicals in soil after clean-up of
	Uranium Mill Tailings Remedial Action Project Sites.
DITTY	Determine the collective dose from long term nuclear waste disposal
1	sites resulting from ground water pathways.
DOSES	Estimates of long-term dose to man from buried waste.
GENII	Internal dosimetry from chronic and acute radiation exposure.
GEOTOX	Evaluated health risks presented from the presence of TNT, RDX and
	benzene present in military explosives residuals.
GWSCREEN	Developed for assessment of ground water pathway from leaching of
	radioactive and nonradioactive substances from surface or buried
	sources.
HHEM	Assist RPMs to develop preliminary remediation goals at CERCLA
	sites.
HRS-1	Hazard ranking for SUPERFUND site assessment.
IMPACTS	Estimates radiological impacts for a given combination of waste
(PART 61)	streams and processing options, disposal technology alternatives, and
	disposal site environmental settings. Used during the development of
	10 CFR Part 61 rule.
MEPAS	A risk computation system developed for hazard ranking applications.
MILDOS	Computes environmental radiation doses from uranium recovery
	operations
MILDOS-AREA	The MILDOS-AREA code provides improved capability for handling
	large area sources and updates the dosimetry calculations.
MMSOILS	Multimedia landfill model.
	EPA Toxicity Characteristic Final Rule.
NUREG 0707	Estimates site-specific limits for allowable residual contamination.
NUREG 5512	Provides generic and site-specific guidance of radiation doses for
	exposures to residual radioactive contamination after the
	decommissioning of facilities licensed by the NRC.
NUTRAN	Calculates the consequences of ground water releases of radioactivity
	from a waste repository.
ONSITE/MAXI1	NRC review of license applications for onsite disposal of radioactive
	wastes.
PATH	Used to implement residual radioactive material guidelines during
PATHI	Models the physical and biological processes that result in the
	transport of radionuclides through the Earth's surface environment
	and eventual numan exposure to these radionuclides.
PATHKAE (-EPA)	Maximum annual effective dose equivalent to a critical population
	group and to ottsite populations at risk from the land disposal of
	Lond to evolute the encoded that a barrie of a standard to stand the standard to standard
PU GEMS	Used to evaluate the spread of toxic chemicals released to air, soil,
	I SUITALE WALEI AILU ULUULU WALEI.

Table 3.2 cont'd - Examples of model usage.				
PRESTO-EPA	Simulates transport of low-level radioactive waste material from a			
	shallow trench site and assesses human risks associated with such			
	transport. This model was modified and added to create the PRESTO			
	family of models.			
PRESTO-EPA-	This is a modified version of PRESTO-EPA-POP. Additions to this			
BRC	model include estimation of radionuclide transport and exposure to			
	workers and visitors, population exposures from incinerator releases,			
	worker and visitor gamma exposures, and onsite farming.			
PRESTO-EPA-	Maximum whole body dose to critical population groups from land			
CPG	disposal of low-level radioactive waste by shallow and deep methods.			
PRESTO-EPA-	Cumulative population health effects to local and regional basin			
POP	populations from low-level waste disposal by shallow land methods.			
PRESTO-EPA-DEEP	Cum. population health effects to local and regional populations from			
	land disposal of low-level radioactive wastes by deep methods.			
PRESTO-II	Evaluation of possible health effects from shallow-land and waste			
	disposal trenches.			
RESRAD	An analytical methodology recommended by the Department of			
	Energy in its guidelines for allowable concentrations of residual			
	radioactive material in soil encompassed by the Formerly Utilized			
	Sites Remedial Action Program (FUSRAP) and Surplus Facilities			
	Management Program.			
RISKPRO	Used to evaluate the spread of toxic chemicals released to air, soil,			
	surface water and ground water. RISKPRO was adapted from			
	PCGEMS.			
SARAH2	Core equations were developed in support of the EPA "Land Disposal			
	Banning Rule."			
UDAD	UDAD provides estimates of potential radiation exposure to			
	individuals and to the general population in the vicinity of a uranium			
	processing facility.			
UTM-TOX	A multimedia model which links an atmospheric transport model with			
	I a surface water model.			

Table 3.3 Evaluations of some other representative multimedia models.										
	Exposure Pathways					Administrative Issues				
				Inhalat	ion		<u> </u>			
			Plant,			<u>† </u>	Current/	Validated/		Available
	External	Soil	Meat, Milk			Ground	Planned	Peer-	Site Data	Computer
Model Name	Exposure	Ingestion	Ingestion	Particulates	Radon	Water	Use	Reviewed	Required	Code
DECHEM			X			X	X		_	X
GENII	X		X	X	X		X	X	Moderate	X
GWSCREEN			X	X	X					X
MEPAS	X	X	X	X	X	X		X	Extensive	X
MMSOILS			X	X		X				X
MULTIMED				X		X	X	X	X	X
NUREG 5512	X	X	X	X		X			Moderate	
ONSITE/MAXI1	X		X	X		X	X	X		X
PATHRAE	X		X	X	X	X	X		Moderate	X
PRESTO-EPA-BRC	X				X	X				X
PRESTO-EPA-CPG	X	X	X	X		X	X	X	Moderate	X
PRESTO-EPA-POP	X	X	X	X		X	X	X	Moderate	X
PRESTO-II	X		Х	X		X	X	X	Moderate	X
RESRAD	X	X	X	X	X	X	X	X	Moderate	X
RISKRPO	X	X		X						X
SARAH2						X				X

4. SOURCE TERM

4.1 Introduction

This chapter deals with the identification and estimation of the source term. The source of emissions and its physical characteristics must be identified before using any model. Source term estimates are provided either by the user, calculated by the model, or back-calculated from measured concentrations at the receptor. Source term conservation entails mass balance calculations to ensure that mass is conserved among multiple release pathways.

4.2 Model Comparisons

4.2.1 Source type

Table 4.1 summarizes possible source types. MEPAS has the most varied selection of source terms, including simulation of injection wells, underground tanks, landfills, lagoons, direct subsurface injection of wastes from tanks or wells, and trenches with caps. Furthermore, MEPAS is the only one of the three models reviewed that allows the user to specify any mass-flux, time-varying distribution of the source term. MMSOILS has a variety of source terms also, but not surface impoundments, direct injection to wells, or trenches with caps. PRESTO-EPA-CPG has the capability of modeling a variety of source terms including waste burial in capped trenches, contaminated soil with and without cover, landfill, and waste piles. None of these models account adequately for the presence of free phase or residually-saturated material in the source terms. Neither do any of these models have the ability to consider facilitated transport, an especially important factor in the transport of radioactive species.

		Capability	
Contaminant Source	MEPAS	MMSOILS	PRESTO
contaminated soil	yes	yes	yes
injection well	yes	no	yes [.]
landfill	yes	yes	yes
surface impoundment	yes	yes	no
trench with cap	yes	no	yes
underground storage tank	yes	yes	no
waste pile	yes	yes	yes

1. PRESTO-EPA-PILCPG considers a source term in a pile.

2. PRESTO-EPA-DEEP

4.2.2 Estimation of the source term

Estimates of the source term are provided either by the user, or are calculated internally by the computer. For example, the release rate of a contaminant spilled on the ground is calculated from the contaminant's vapor pressure, soil/vapor partitioning.

and molecular diffusion in air. The PRESTO-EPA-CPG model does not consider the vaporization of radionuclides, and assumes that all contaminants will be transported either through atmospheric pathways in absorbed form or through water pathways in dissolved form. The fate of release through water pathways is calculated internally from the mass-balance equation using the inventory and leaching/solubility characteristics of the given radionuclide and the internally calculated stream flow. In applications to radioactive waste disposal, this approach will give conservative results for health risk assessments always, especially when the chemical forms of the contaminant are unknown.

For the atmospheric component only, MEPAS has the option of back-calculating release rates from measured concentrations at the receptor. This requires data on (i) air concentration, (ii) soil concentration, or (iii) both. This option is not available in the other two models.

4.2.3 Conservation of the source term

Since the individual pathway models in MEPAS, MMSOILS, and PRESTO-EPA-CPG are linked implicitly, verifications of mass conservation are needed to prevent multiple accounting of the same mass of contaminant in different media. MEPAS accounts for depletion of the source via a link between the source's inventory and release rate and duration that ensures that a release is over. This option addresses the theoretical need for mass conservation, but is useful only when the inventory of the source is known. Sometimes there is more certainty about the duration of the release and the inventory than about the rate of release. When the inventory of waste is uncertain, great care is needed in using the source depletion option properly, especially for long-term simulations (Peer Review Committee report, 1994).

MMSOILS includes calculations of mass balance annually to ensure that mass is conserved in waste management units that have multiple release pathways. These calculations compute the accumulation and depletion in landfills, impoundments, and waste piles. For each unit, the mass that is removed from each pathway is accounted for annually, to satisfy overall mass conservation.

PRESTO-EPA-CPG includes mass-balance calculations also to insure that mass is conserved in waste management units. This equation calculates the rate of release and the mass remaining in the waste units. Then, the radionuclide mass is adjusted for the radioactive decay at the end of each year.

4.2.4 Air pathway

4.2.4.1 Air source

MEPAS has an option allowing the user to specify a uniform ambient concentration of the contaminant as a source term when there are measurements of the ambient concentration of the contaminant at a waste site. A similar option is provided in PRESTO models. A user-assigned strength of background radionuclide concentration in the atmosphere above the contaminated area can be added to the resuspended radionuclide concentration for assessing the combined health effects. MMSOILS does not have this option.

4.2.4.2 Radioactive and chemical decay

MEPAS can handle both first-order radioactive and chemical decay, while MMSOILS is limited to chemical decay. Progeny formation is not calculated in MMSOILS. MEPAS handles progeny formation in ground water, surface water, surface soil, and deposited contaminants from wet and dry deposition, but not while the contaminant is moving in the air; it handles it after the contaminant has been deposited. The PRESTO-EPA-CPG model calculates radiological effects for the progeny produced by up to a four-member decay chain.

4.2.4.3 Volatilization from soil or spill

In both MEPAS and MMSOILS, volatilization is calculated by either steady-state or transient equations, depending on the scenario of release (Table 4.2). Steady state equations are used in scenarios of landfill release and sediment-controlled emissions, whereas time-averaged solutions of transient diffusion equations are used for releases from spills, contaminated soil, and land treatment facilities. The steady-state equations assume a very large source, so that emission does not deplete the source during the time considered.

In the MEPAS scenarios of releases from spills and land treatment facilities, the volatilization flux is calculated by accounting for the decrease over time of the concentration of the chemical in the soil. A dry-out period is computed, after which emissions stop. MMSOILS does not define explicitly a similar mechanism of tracking and depletion.

PRESTO-EPA-CPG assumes that all volatile radionuclides are released in a water-soluble form and contribute to the ground water and surface water pathways. PRESTO-EPA-CPG was designed primarily for use at low-level radioactive waste disposal sites, and assumes that the health effects due to the volatile radionuclides (primarily ¹⁴C and ³H) are negligibly small. PRESTO-EPA-CPG is not included in Table 4.2. for this reason.

Table 4.2 Source term of volatilization scenarios.						
	Submodel	Assumptions				
No	Description	MEPAS	MMSOILS			
1	Landfill, without gas generation/ (Farmer's Equation Covered Sites)	 Steady state Very large source (emission does not deplete source during time frame considered) 	Same as MEPAS, but steady-state flux is limited by mass inventory			
2	Landfill, with gas generation (Municipal Waste)	 Steady state Very large source (emission does not deplete source during time considered) 	NA			
3	New spill	 Time-averaged form of transient solution, emission rates decrease with time Emissions occur from liquid above spilled surface A dry-out period is computed, after which emissions stop. 	NA			
4	Old spill (Covered Sites. Adsorbed Phase)	 Time-averaged form of transient solution; emission rate decreases with time Contaminant concentration in cover soil initially is zero; uniform concentration underneath cover to finite depth Vapor concentration at soil surface is maintained at zero Release rate controlled by soil/vapor partitioning and molecular diffusion in air A dry-out period is computed, after which emissions stop. 	•Release rate controlled by soil/vapor partitioning and molecular diffusion in soil gas (i.e., controlled by diffusion of vapor in a porous medium, which is 1-2 orders of magnitude less than diffusion in air.			
5	Soil Contaminated up to the Surface/ (Uncovered Sites, Adsorbed Phase)	 Time-averaged form of transient solution; emission rate decreases with increasing time Release rate controlled by soil/vapor partitioning and molecular diffusion in air 	Same as MEPAS			
6	Contaminated Soil covered with a layer of Clean Soil/ (Covered Sites, Adsorbed Phase)	 Same assumptions and equations as submodel 4 above 	Same as MEPAS			

1. Submodel descriptions in *italics* refer to MMSOILS.

Table 4.2 cont'd Source term of volatilization scenarios.			
	Submodel	Assumptions	
No	Description	MEPAS	MMSOILS
7	Land Treatment Facilities/ (<i>Landfarming Equation</i>)	 Time-dependent release rate Release rate controlled by liquid-phase concentration of contaminant in soil Contaminant concentration is constant until all its mass vaporizes from liquid-phase 	Same as MEPAS (slightly different equation for release rate)
8	Sediment-Controlled Emissions	 Steady state Includes both sediment-to-water and water-to- air transfer; mass transfer coefficients control diffusion in the two media 	Same as MEPAS
9	Surface impoundments, e.g. ponds, lagoons, small lakes./ (Volatilization from a Contaminated Water Body)	•Two-layer resistance model; a gas and a liquid film across the air-water interface form the dominant resistance to mass transfer	Same as MEPAS (model not yet in code) ²
	General	 Emission rates of low-volatility contaminants are constant during time considered Emission rates of highly volatile contaminants 	
		decrease significantly with time; thus, ambient concentrations are computed mainly as a function of total amount of released material rather than emission rate. User determination of contaminant's total inventory is crucial for highly volatile materials	

1. Submodel descriptions in *italics* refer to MMSOILS.

2. A model of volatilization from contaminated water is described in MMSOILS manual, but is not included in the 1993 computer code. See Model Developer's Comments - Section 4.3.2.

4.2.4.4 Air-borne depletion due to deposition

All models account for airborne contaminant depletion via dry deposition. Wet deposition and the associated source depletion is included in MEPAS and PRESTO-EPA-CPG, but not in MMSOILS.

4.2.5 Ground Water Pathway

4.2.5.1 Generation of leachate

Contaminants are introduced into the ground water pathway from leachate originating in a waste management unit. Leachate migrates vertically through the unsaturated zone and discharges finally into the saturated ground water system. The way in which leachate is generated is similar in the three models.

MEPAS contains the most sophisticated source term for leachate of the three codes. MEPAS was set up specifically to permit the user to define the source term if it is known. The user specifies the total inventory of waste in the unit and the leaching rate. The code has a mass-balance check to see that there is enough inventory to match the amount of material leached from the source.

If the user cannot define the source term, MEPAS will calculate it based on a combination of: (i) solubility limit on concentration, (ii) equilibrium partitioning with contaminated soils, (iii) steady-state concentration of leachate supplied by user, and (iv) transient or time-varying releases as specified by user.

MEPAS provides the user with three source term options:

Option 1: the user supplies the source term concentration; the code supplies the rate of deep-drainage percolation; then, the code calculates the time-varying mass-flux rate. This information can be supplied for a point source, line source (accounts for both the x and y directions), or area source. The source can be a ponded site or a contaminated-soil site. The movement of the contaminant can be released directly to the vadose zone and then, to the saturated zone, or it can be released directly to the saturated zone. Operational releases and non-operational releases (i.e., past-practice sites) are considered.

Option 2: the user supplies time varying mass-flux rate from the source and the rate of deep-drainage percolation; then the code calculates the initial source term concentration. This information can be supplied for a point source, line source (accounts for both the x and y directions), or area source. The source can be a ponded site or a contaminated-soil site. The movement of the contaminant can be released directly to the vadose zone and then, to the saturated zone, or it can be released directly to the saturated zone. This includes direct discharge (e.g., injection well, pipe to a river) also. Operational releases and non-operational releases (i.e., past-practice sites) are considered.

Option 3: a combination of Options 1 and 2.

MMSOILS was designed specifically to address leaching from landfills and waste piles. The leachate can be generated from soil, landfills, waste piles, surface impoundments, and underground storage tanks (USTs). In the first three, the contaminants are dissolved in infiltrating recharge water derived from precipitation. By definition, surface impoundments contain pre-mixed leachate that infiltrates into the unsaturated zone. MMSOILS uses a continuously mixed reactor model for this source type.

Like MEPAS, MMSOILS has several different options for generating leachate for landfills and waste piles: (i) solubility limit on concentration of leachate, (ii) equilibrium partitioning with contaminated soil, (iii) completely mixed reactor, and (iv) steady-state concentration of leachate specified by the user. Thus, the user can choose from a variety of options, depending upon how much data are available for the site. If the data are limited, the steady-state option allows the user to specify a concentration of leachate.

PRESTO-EPA-CPG can model leachate source terms from ground surface contaminated soil, waste trenches with cover, and waste piles. It has similar options for generating leachate to those of MMSOILS: (i) solubility limit on the concentration of leachate, (ii) equilibrium partitioning with contaminated waste mixed with soil, and (iii) release fraction. The latter is similar to the steady-state option of MMSOILS.

Since landfill leachate is known to contain high concentrations of colloids that are likely to facilitate the transport of radionuclides, it is especially significant that none of these models can consider such facilitated transport.

4.2.5.2 Other source terms

MEPAS and another version of PRESTO-EPA (-DEEP) have additional source terms for ground water in the form of injection wells. The user specifies both the concentration of contaminant in the injected water and the flow rate. MMSOILS does not have this source term.

4.2.6 Surface Water Pathway

4.2.6.1 Soil erosion

MMSOILS and MEPAS allow erosion of the contaminated soil from the waste unit. Then the soil is transported into the surface water where it continues to act as a source of dissolved contaminants. The contaminants are dissolved into surface water using an equilibrium partitioning approach. In the scenario of the source term in shallow trenches with cover, the PRESTO-EPA-CPG model assumes that the cover is constructed with clean soil. Therefore, the eroded soil will not contain contaminants as long as the cover remains effective (i.e., as soon as the cover is eroded) the contaminants would begin to dissolve into the surface runoff water and be transported away from the contaminated unit. When there is no cover, the PRESTO-EPA-CPG model assumes that the contaminants will be transported into the surface water body as soon as erosion begins. Thus, the surface water body will be contaminated from the beginning of the simulation. An equilibrium partitioning model using a linear sorptiondesorption relationship is used also in calculating the rate of transport of contaminants.

4.2.6.2 Runoff

All three codes allow rainfall to leave the unit as runoff. They assume that the runoff water is in chemical equilibrium with the contaminated soil, using a simple partitioning model. The assumption that runoff water will be in chemical equilibrium is an oversimplification. The degree to which runoff water achieves equilibrium will rely on the partitioning coefficients and the residence time of surface water in contact with the contaminated surface soils. In most scenarios, there is likely to be far less time than is required to achieve chemical equilibrium. As such, this assumption will be overly conservative.

4.2.6.3 Ground water inflow

All three codes allow the interception of the contaminated ground water by a surface stream. A complete mix (also called a "completely mixed") model is assumed by MMSOILS and PRESTO-EPA-CPG as the ground water enters the surface. MEPAS does not assume a completely stirred tank reactor (a CSTR, operationally the same as a complete mix model), but uses a plug-flow with dispersion model (i.e., a solution to the advective-dispersive equation). Such a model accounts for plume migration in the lateral direction from the bank where the source enters the stream.

4.3 Developer Updates - Source Term

4.3.1 MEPAS

Droppo (1994) reports that MEPAS Version 3.0 has the capability of direct input of waterborne monitoring data in computing risk values. A module to include geochemistry in the environmental release component of MEPAS is being developed also. The new source term code for MEPAS will provide a coupled contaminant source term that is partitioned to the different environmental media for transport and exposure. Two- and three-dimensional, spatially-varied concentrations for any designated period will be implemented in MEPAS. Thus, MEPAS will be able to calculate the contribution to downgradient sites from multiple waste sites.

4.3.2 MMSOILS

The most recent version of MMSOILS contains a two-layer resistance model for air-water interface transfer (see item 9 Table 4.2).

4.3.3 PRESTO-EPA-CPG

Future versions of PRESTO-EPA-CPG will contain an improved infiltration submodel for handling uncovered contaminated soil (Hung, 1994).

5. AIR TRANSPORT

5.1 Introduction

The air-transport pathway is one of the principal pathways whereby radionuclides released from waste sites may reach living organisms. Radionuclides may be discharged to the atmosphere through particulate suspension, venting from containers, and volatilization from contaminated water and soil. Once airborne, they will disperse downwind and deposit on ground surfaces in a pattern dependent on the local meteorology, the location of the point of release, the nature of the terrain downwind of the release, and the physical and chemical characteristics of the emission. Exposure to humans can occur via direct radiation, inhalation, or consumption of contaminated water, crops, and animals (Figure 5.1).





The objective of atmospheric transport modeling is to predict the concentration of radionuclides at specific locations surrounding the source. The basic types of data required to run these models include the release rate of each radionuclide, physical characteristics of the source (e.g., stack height, area, or release). and meteorological data (e.g., stability class, wind speed, precipitation). For environmental radiological assessments, models should be able to simulate plumes from point sources (e.g., containment leaks) and area sources (e.g., contaminated ponds), for several minutes up to several years, and up to about 80 km from the source. Also, these models should

include volatilization from soil and water, and particulate emissions from wind erosion and mechanical operations. As the plume travels downwind, it disperses in the air and is depleted also by deposition to ground surfaces, radioactive decay, and chemical decay. Such depletion processes are important for radiological health assessment. The outputs from these models include the concentration of air and surface contaminants which can be used in assessing the inhalation and ingestion components of the exposure. The surface contaminant levels are used also as input to the overland transport pathways. Figure 5.2 shows these interactions.



Figure 5.2 Diagram of pathway interactions (after Droppo et al., 1993).

5.2 Comparisons of models

The same sector-averaged Gaussian plume equation for air transport is used in all three models. Most of the volatilization algorithms in MEPAS and MMSOILS are also the same. However, MMSOILS and PRESTO-EPA-CPG do not describe complex

terrain effects, calms, wet deposition, and contaminant decay. In addition, PRESTO-EPA-CPG does not include several components such as area releases and volatilization from lagoons, lakes, ponds, and rivers, and the suspension of particles due to loading and unloading operations.

5.2.1 Radioactive and chemical decay

Depletion of radionuclides in the plume by radioactive decay may be significant when the decay is fast (e.g., emissions of cesium, iodine, manganese, radon, and ruthenium) and transport is slow. This option is available in PRESTO-EPA-CPG, but not in the current version of MEPAS or MMSOILS. MMSOILS can model first-order chemical decay once the contaminant is deposited on soil, but not radionuclides explicitly. None of these models describes the creation of progeny within the air pathway.

5.2.2 Wet deposition

Ground deposition can result from wet and dry processes, and for many locations the magnitude of these processes in depleting airborne radionuclides is roughly the same. Wet deposition is caused by rain scavenging the contaminant and by deposition of cloud droplets which have absorbed the contaminant. Dry deposition is the direct deposition of the airborne contaminant onto a surface by gravitational settling, or impacting. Ground deposition is necessary for linking the air-pathway models with the water and food chain models. Wet deposition is included by MEPAS and PRESTO-EPA-CPG, but not by MMSOILS. Therefore, MMSOILS will underestimate ground concentrations and overestimate air concentrations, with the error increasing with the distance from the source.

5.2.3 Air source

Chapter 4, section 4.2.3.1 discusses the air source term for the three models.

5.2.4 Calm conditions

Calm conditions can be extremely important in assessing health impacts to populations near the source (e.g., up to 10 km). In some locations, the prevailing winds blow from one direction, and calms (e.g., wind speeds <1m/s) from another direction. If calms occur often, they can cause much higher concentrations at near-field receptors than predicted by the wind-rose data. The effect of calm conditions is more important in determining acute effects than long-term ones as such conditions may change over long periods. MEPAS can distribute calms as a function of direction, and models them with a wind speed of 0.5 m/s. Calm conditions are not described by the other two codes.
5.2.5 Complex terrain

The atmospheric pathway in MEPAS takes into account local site influences in a highly simplified manner and describes complex terrain characteristics such as channeling in a valley, and intersection with hills around a release. PRESTO-EPA-CPG and MMSOILS account only for different roughness of a flat terrain. In general, complex terrain adjustments have more effect on maximum individual exposures than on average population exposures. However, in sites where the flow of contaminants towards surrounding receptors is either interrupted or concentrated by hills or valleys, these topographical features can affect average population exposures significantly.

5.2.6 Acute effects

MEPAS calculates maximum (hourly) air concentration and its location in each direction to determine acute effects; the other two models do not. All three atmospheric pathway models use annual averages, and predict annual average concentrations and subsequent exposures. Average annual exposures might not represent adequately strongly seasonal (e.g., calm conditions) or event-driven (e.g., large storms) environmental transport. MEPAS includes equations necessary to describe such variations, but its present structure is limited to the calculation of annual estimates.

The features of these models and their fundamental assumptions are further described in Table 5.1.

5.3 Developer Updates - Air Transport

As reported by Droppo (1994), a planned update of MEPAS will compute a single mass budget for airborne-waterborne releases rather than separate mass budgets.

Table 5.1. Atmospheric pathway: Comparison of capabilities.					
	Submodel	Availability & Fundamental Assumptions			
No	Description	MEPAS	MMSOILS	PRESTO-EPA-CPG	
1	Point Releases	yes	no	yes	
	Ground	Sector-averaged Gaussian	no	Sector-averaged Gaussian	
	Elevated	Sector-averaged Gaussian	no	Sector-averaged Gaussian	
	Plume rise	Briggs, 1975	no	yes	
2	Area Releases	Approximation with point source	Approximation with point source	user input C/Q and sector	
{ .		at virtual distance and sector	at virtual distance and sector	averaged Gaussian plume	
		averaged Gaussian plume	averaged Gaussian plume		
	Sail	yes	yes	yes	
[Landfills	yes	yes ¹	yes	
	Lagoons	yes	yes1	no	
	Lakes, ponds, rivers	yes	yes ¹	no	
	Multi-point regional	no	no	no	
3	Suspension of particles	Sehmel, 1976; Cowherd et al,	Sehmel, 1976; Cowherd et al,		
		1989	1989	<u> </u>	
L	Wind speed	yes	yes		
[Surface roughness (z)	0.1 <z<1000 cm<="" td=""><td>yes</td><td>yes</td></z<1000>	yes	yes	
L		snow to high-rise bldgs			
	Mechanical disturbance	yes	yes	yes	
	Loading & Unloading	no	yes	no	
	Soil spreading operations	no	yes	yes	

no = Not available, yes = Available

1. A model of volatilization from contaminated water is described in MMSOILS manual, but is not included in the 1993 computer code. It is coded in the most recent version of the model - see Developer Updates (Section 4.3.2).

2. Code to handle multi-point regional releases has been written for MEPAS, but is not provided on the distribution disks. This capability has been used only in efforts conducted by Pacific Northwest Laboratory.

6. GROUND WATER TRANSPORT

6.1 Introduction

Often, ground water is an important pathway for wastes found below the land surface. Contaminants leach from the waste, move downward through the unsaturated zone to the water table, and then migrate in the saturated ground water system. The contaminants may discharge ultimately either to a drinking water well or to a surface stream (Figure 6.1). Humans are exposed to radioactive and other contaminants by using well water or surface water, and by eating organisms living in the surface streams.

The ground water component of multimedia models predicts the concentration over time at wells and surface discharge areas. Usually, these calculations are broken down into three linked sub-pathways: (i) leaching of contaminants from the waste unit, (ii) vertical movement of the dissolved contaminant downward to the water table through the unsaturated zone, and (iii) migration of the contaminant in saturated ground water to the receptor point. Separate models simulate these three processes, with the preceding model supplying a source of contaminated water to the next one. Thus, the leachate generation model supplies a source of contaminated water to the unsaturated zone model, which passes the contaminated water subsequently to the saturated ground water model at the water table.

Ideally, these models would be three-dimensional, capable of incorporating all our knowledge of the subsurface, and of simulating the complex chemical reactions that occur as the contaminant migrates through the soil and aquifer materials. Unfortunately, even the most sophisticated ground water models cannot address all these issues. Since multimedia models are used often as screening tools or for comparing different sites, each pathway is simplified to incorporate only the most basic features. Furthermore, these features must be described with limited data. For the ground water pathway, most multimedia models simplify the unsaturated zone to a onedimensional (1D) model which assumes that the contaminant migrates only vertically from the waste source to the underlying water table. In most cases, this is a valid assumption because the scale of transport in the unsaturated zone tends to be orders of magnitude smaller than that in saturated ground water.

Further simplifications are made for the saturated ground water model. The most common assumptions are that ground water moves at a uniform rate and is unaffected by pumping wells, changes in recharge, or other systems stresses. These assumptions are much less realistic than the simplifications made to the unsaturated zone models, but for screening they are adequate as long as the user understands the degree of uncertainty in the model's results. The following disclaimer from the MMSOILS manual is a good synopsis of the problems inherent in this approach:

"It is important to be cognizant of the uncertainty inherent in this type of model. Often the most basic parameters, such as contaminant concentration in soil, vary significantly over a given site and the distribution may be poorly understood. These uncertainties, coupled with approximations that were used to streamline the modeling process lead to results that may differ from reality by orders of magnitude. As such, the user is cautioned to examine the input and output of the model closely and consider a sensitivity study to evaluate the impact of varying input parameters on the calculated results."

6.2 Comparisons of Models

Table 6.1 outlines a range of capabilities for modeling the ground water pathways. The approach to modeling the ground water pathway in MEPAS (Whelan et al. 1987) and MMSOILS (U.S. EPA, 1992) is similar. However, PRESTO-EPA-CPG (U.S. EPA 1987) differs from the other two codes in many ways which are enumerated below.



Figure 6.1. Conceptual diagram of the ground water pathway (Whelan et al. 1987).

6.2.1 Radioactive decay/progeny ingrowth

Each model incorporates a first-order decay coefficient to simulate decay. While MMSOILS is not specifically designed to consider radioactive decay, it does incorporate a decay term for non-radioactive chemicals. However, MMSOILS limits the decay to dissolved chemical contaminants; which when adsorbed onto the soil material do not undergo decay. While this is a conservative assumption which would lead to persistence of the chemical contaminant in the environment, it is overly conservative since many radionuclides are strongly sorbed onto most soils.

Only MEPAS and PRESTO-EPA-CPG simulate ingrowth of progeny during decay; this may be important if travel times in ground water approach the half-life of the contaminant, or if the progenies are particularly toxic, or if the progeny is in a different physical state (e.g., radium to radon).

MEPAS assumes that the progenies have the same distribution coefficient (K_d) as the parent. This is seldom the case and should be considered when reviewing the output from MEPAS for scenarios where progeny ingrowth is important. This drawback is only significant when the parent nuclide has a short half-life or when the travel time is long relative to the parent's half-life. The NRC NUREG-0868 states that " the assumption of equal transport speeds makes a relatively small difference to the calculation of concentrations of the most important components, and is conservative." The user always has the option of modeling the decay products as parents instead of, or in addition to, the actual parent radionuclides, thereby bounding the problem without making any assumption about K_ds .

There are two versions of PRESTO-EPA-CPG available for simulating progeny ingrowth: a research model and a screening model. The screening version assumes that progeny have the same K_d as the parent, while the research version assumes that progeny and parent nuclide may have different ones. The latter model uses the sophisticated mathematical formulations developed by Burkholder and Rosinger (1980). The computation time for this version of the model is several times longer than the model without simulation of progeny ingrowth. This version is used currently only for research because of this extended calculation, and because the PRESTO-EPA-CPG model is designed as a screening-type model. The screening version assumes that progeny and the parent have the same K_ds . As a result, the computation time of this version of the model without progeny ingrowth.

Table 6.1 Ground water pathway: Comparison of capabilities.				
Capability	MEPAS	MMSOILS	PRESTO	
Unsaturated Zone				
Miscible Transport	yes	yes	yes	
Model Type	1D semi-	1D finite-	1D	
	analytical	element	analytical	
Advection	yes	yes	yes	
Dispersion	yes	yes	no	
Diffusion	yes	no	no	
Physical/Chemical Processes				
Decay	yes	yes	yes	
Progeny Ingrowth	yes	no	yes	
Sorption	linear	linear	linear	
Other Chemical Reactions				
Immiscible Transport	no	no	no	
Vapor Transport	yes	no	no	
Saturated Zone				
Miscible Transport	yes	yes	yes	
Model Type	3D semi-	3D semi-	1D	
	analytical	analytical	analytical	
Advection	1D	1D	1D	
Dispersion	3D	3D	2D	
Diffusion	3D	no	no	
Physical/Chemical Processes				
Decay	yes	yes	yes	
Progeny Ingrowth	yes²	no	yes	
Sorption	linear	linear	linear	
Other Chemical Reactions	no	no	no	
Immiscible Transport	no	no	no	
Density-Dependent Flow	no	no	no	
Fractured Zone	no	no	no	

1. No decay occurs while contaminant is sorbed onto soil.

2. Progenies have the same adsorption coefficients (Kd) as parent.

3. MEPAS handles vapor transport within the air model.

6.2.2 Unsaturated zone model

Each of the three codes includes an unsaturated zone model which simulates transport of the dissolved contaminant from the waste source downward to the water table. All the models use a one-dimensional approach, which is acceptable usually except when the unsaturated zone is extremely heterogeneous. At most sites, data are not collected routinely to support more complex simulations of unsaturated flow and transport. Therefore, the use of a one-dimensional model is not a limiting factor.

MMSOILS provides the most complex model of the unsaturated zone of the three codes. It uses a one-dimensional, finite-element flow and transport model that allows for layered heterogeneity in the unsaturated zone. The finite-element model is the

same model (VADOFT) as that used in Rustic (USEPA, 1989), a more complex subsurface simulator.

MEPAS uses a one-dimensional, semi-analytical transport model that assumes a constant vertical velocity for each layer in the vadose zone. The user may describe the vadose zone with multiple layers. Therefore, the user can account for heterogeneity in the vadose zone by modeling multiple vadose-zone layers with velocity variability between layers, and infiltration rates that change with time. MMSOILS, with its layered finite-element model computes a non-uniform vertical velocity based upon changing soil properties.

PRESTO-EPA-CPG uses an empirical formula developed by Clapp and Hornberger (1978) to calculate the average degree of saturation which then is used to obtain the unsaturated water velocity and retardation factor. Then, the rate of radionuclide transport is calculated from a steady-state, one-dimensional transport equation.

6.2.3 Saturated Zone Model

MMSOILS and MEPAS take similar approaches to simulating transport of contaminants in the saturated ground water flow, using a three-dimensional, semianalytical transport model. The three-dimensional adjective is somewhat misleading, however, because only dispersion is considered in three dimensions. Ground water velocities are assumed to be uniform and horizontal, and thus one-dimensional. The codes used in these semi-analytical transport models are similar to the AT123D code (Yeh, 1981).

Both the MEPAS and MMSOILS mathematical formulations employ a convolution integral that distributes a transient release from the source to the receptor, thereby avoiding problems with convergence and instability since each time step is calculated independently of its predecessor. Short (i.e., 1 year) or long (i.e., 10 million year) simulations are possible without the risk of problems of instability or convergence because the user-defined time steps are independent. A potential problem may occur with this integration scheme if the upper and lower bounds and limits of integration are not properly selected.

The PRESTO-EPA-CPG model employs a simple one-dimensional model (Hung. 1986) to achieve the goal of analyzing the annual rate of radionuclide transport for 10,000 years. Although an analytical model, PRESTO-EPA-CPG can adopt any form of boundary conditions and can consider lateral and longitudinal effects. It is designed as a screening-type model, aiming at an accurate health-effects evaluation with a minimum of numerical calculations. To achieve these goals, a correction factor, called Hung's correction factor compensates for the rate of radionuclide transport obtained from the analytical model without lateral dispersion effects (Hung, 1986). Since Hung's correction factor is derived by matching the total mass of radionuclides passing through a particular layer, theoretically, the estimated cumulative health effects should agree

with the results obtained from a numerical approach. As to the maximum dose analysis, the solution using Hung's model and that using a numerical approach are fairly close, in general, to each other as long as the transport number is less than 4 and the Peclet number is greater than 2 (Hung. 1986). In a general waste disposal site risk assessment application, the transport number and the Peclet number are usually within the domain described above. Therefore, the PRESTO-EPA-CPG model can calculate the maximum individual dose with minimum error compared to the exact solution obtained from a one-dimensional model.

6.2.4 Mixing-zone calculations

The results of the unsaturated zone model are a flux of contaminants that serve as a source term for the saturated zone model. The volume of aquifer over which the contaminant flux is diluted when it first enters the aquifer is called the mixing zone. Each model treats the mixing zone differently. The least conservative approach is to mix the contaminants over the entire saturated thickness of the aquifer, as is done in PRESTO-EPA-CPG. That approach causes maximum dilution, resulting in the lowest possible concentration of contaminants in the saturated zone beneath the source. However, the unsaturated zone concentration can be concentrated rather than diluted, as occurs when the water flow from the unsaturated zone into the aquifer exceeds the ground water flow out of the source.

MMSOILS computes the vertical dispersion coefficient and a mixing depth, called the depth of penetration, using the ratio of the horizontal rate of ground water flow to the vertical flow-rate of water from the unsaturated zone. As the amount of vertical flow and the vertical dispersivity increase, the thickness of the mixing zone increases.

MEPAS assumes that the flux of contaminants occurs at the water table and the depth of mixing depends directly upon the vertical dispersivity value.

Both MMSOILS and MEPAS assume that the pumping of a well does not affect the background flow of ground water. This assumption is applicable only when the unit-width flow strength is much greater than the pumping rate. However, a waste disposal or cleanup site may be situated in a region of low or moderate ground water flow, a situation that would disqualify this assumption. In such a region, a well screen would be set near the bottom of the aquifer and pumped with several times higher capacity than the daily demand. In most cases, this would create a free surface drawdown in the vicinity of the well, so that the contaminant plume will be pulled down and mixed with the bottom layer of clean water. Although this mixing may occur only in the vicinity of the well, the quality of water being pumped out would be close to complete mixing. For these reasons, the assumptions of the PRESTO-EPA-CPG model may be reasonable.

6.2.5 Adsorption of contaminants

All three models assume a linear, fully reversible, adsorption model in both the unsaturated and saturated zones. The only difference between them is that MMSOILS assumes that contaminants do not decay while sorbed to the soil matrix.

6.2.6 Complex processes

None of the models simulate complex transport processes, such as vapor phase transport, fracture flow, or immiscible phase transport. At a particular site, these processes may be important. For example, transport of radon in soil gas may be important for exposure assessments, if radium is one of the contaminants of concern.

6.2.7 Requirements for data input

The requirements for data input in MMSOILS (Table 6.2), MEPAS (Table 6.3), and PRESTO-EPA-CPG (Table 6.4) differ significantly. MEPAS requires the most data, especially for the soil and unsaturated zones. A data-input guide is provided that explains each parameter and gives suggestions on selecting a value for a parameter. One problem with this guide is that metric and English units are mixed. For example, hydraulic conductivity is entered in units of ft/d, while bulk density is expressed in g/cm³. According to the developers, the default units employed by MEPAS were chosen to conform with those most likely to be found in data source documents. The data-input shell of MEPAS can be redefined to employ any units (consistent or otherwise) desired by the user, since this model can convert any set of units used.

Modeling the unsaturated zone within MMSOILS could require significantly more data input than the other two models, if numerous soil layers are incorporated in the model (10 data elements are entered for each soil layer). System International (SI) units are used consistently throughout MMSOILS except for time units which are expressed in years for the decay coefficient, and hours for hydraulic conductivity.

PRESTO-EPA-CPG requires very little data for the ground water pathway, consistent with its low sophistication in the subsurface transport models. The units are internally consistent in PRESTO unlike MMSOILS and MEPAS.

6.3 Developer Updates - Ground water Transport

Improved capabilities for ground water transport of light, non-aqueous phase liquids (LNAPLS) and dense, non-aqueous phase liquids (DNAPLS) are planned for future versions of MEPAS according to Droppo (1994). Version 3.0 of MEPAS includes also an improved calculation for waterborne transport that incorporates double-precision mathematical routines to address problems that would

arise because of round-off errors. New versions of MEPAS will account for curvilinear flow in the saturated zone also.

Table 6.2 Data requirements for MMSOILS.
Unsaturated Zone
Climatic Data
pan factor for converting pan evaporation to potential evapotranspirat on
latitude of site
precipitation data (12 months)
number of days with precip. (12 months)
average temperature (12 months)
pan evaporation (12 months)
starting and ending month for growing season
Soil Property Data
curve number of surface soil
field capacity of soil
wilting point of soil
depth of root zone (cm)
number of soil layers (entering the following for each layer)
saturated hydraulic conductivity (cm/hr)
saturated water content
bulk density (gm/cm ²)
exponent "b" for moisture curve
percent organic matter
percent clay
percent silt
percent sand
railo of hist-order decay (1/yr)
(nickness of layer (cm)
Saturated Zone
hydraulic gradient (dimensionless)
hydraulic conductivity (m/yr)
porosity (dimensionless)
bulk density of aquifer material (gm/cm [*])
fraction of organic carbon in aquifer
dispersivity (x, y, and z-directions) (m)
aquiter thickness (m)
1st order decay rate (yr ')
time (yr)
x,y,z locations (meters)

Table 6.3 Data requirements for MEPAS.

Unsaturated Zone depth of waste site in unsaturated zone (ft) length of site (ft) width of site (ft) waste liquid infiltration rate (ft/d) Top Soil Data moisture content of soil bulk density of soil (g/cm^3) soil textural classification percent sand, silt, and clay percent organic content percent iron and aluminum pН percent vegetative cover water capacity SCS curve number Partially Saturated Zone Data soil textural classification percent sand, silt, and clay percent organic matter percent iron and aluminum pН thickness of partially saturated zone (ft) bulk density (g/cm³) total porosity field capacity dispersivity (fl) saturated hydraulic conductivity (ft/d) Saturated Zone soil textural classification percent sand, silt, and clay percent organic matter percent iron and aluminum pH of pore water total porosity effective porosity contaminant velocity (ft/d) thickness of saturated zone (ft) bulk density of saturated zone (g/cm³) travel distance in saturated zone

longitudinal, transverse, and vertical dispersivity (ft)

Table	6.4 Data requirements for PRESTO-EPA-CPG.
Unsatu	irated Zone
	length of contaminated zone (m)
	average slope of contaminated zone
1	component of porosity for gravity water
1	component of porosity for pellicular water
	thickness of the top layer (m)
ſ	equivalent diffusivity (m²/hr)
	maximum day length for each month (hr)
	mean daily temperature (°C)
	hourly rainfall (0.1 mm/hr)
	percentage of top layer failure
1	annual infiltration rate (m/yr)*
	fraction of residual saturation
	distance from bottom of trench to nominal depth of aquifer (m)
	porosity
	nydraulic conductivity (mvyr)
	duik density (g/m²)
Satura	ted Zone
	distance between well and stream (m)
	distance from trench to well (m)
	ground water velocity (m/yr)
	thickness of aquifer (m)
	dispersion angle (radians)
	bulk density (g/m³)
	longitudinal dispersivity (m)
	porosity

* internally calculated, output from transient zone calculation.

7. RUNOFF, EROSION, AND SURFACE WATER TRANSPORT

7.1 Introduction

Surface water may be an important pathway by which contaminants are transported from a waste disposal site; such pathways include lakes, streams, rivers, and the rainfall-runoff process. Contaminants present on the surface of a waste site may become entrained or dissolved in surface runoff and be transported to adjacent bodies of surface water. Contaminated soil particles detached by the impact of rain drops or eroded by surface runoff may be transported to surface bodies also. Exposure to humans can occur then through drinking and using contaminated surface water, or by eating organisms living in these water bodies (Figure 7.1).





The pathways for surface water from a contaminant source to drinking water (or immersion exposure) can be sub-divided into three major components:

- Infiltration into the subsurface and eventual discharge of ground water into surface water bodies
- Runoff across the land surface transporting dissolved, suspended, and bed load as overland flow
- Mixing of the contaminated surface or infiltrating ground water with a surface water body.

The magnitude of each of these components can be predicted using empirical or physically-based equations that model the transport of contaminants through overland and ground water flow to a surface water body. These equations need to consider the following classes of variables:

- The quantity and intensity of precipitation
- The physical characteristics of the soil that control the soil's ability to absorb and transport water and contaminants, including antecedent moisture conditions
- The nature of vegetative cover
- Topographic features of the landscape, such as slope and the presence of depressions
- The physical characteristics of the surface water body into which runoff flows and ground water infiltrates.

The mechanisms by which different radionuclides are transported to surface water bodies usually vary with their respective geochemical properties. Radioactive metals in solution tend to bind to soil components, leaving only a small fraction in solution. Conversely, some radioactive constituents such as tritium tend to remain in solution with only a small fraction binding to soil materials. Consequently, radioactive metals in streams are related to surface runoff (event water) and soil erodibility generally, while more soluble constituents may be related more to infiltration, dissolution, and ground water discharge. It is essential to model processes (flow pathways), in addition to flow amounts, in order to analyze behavior of these and other contaminants in natural systems. This conclusion would imply that physically-based models should produce more accurate predictions for the surface water components than empirically-based models.

Methods for simulating surface water transport fall into two broad categories empirically and physically based. Two examples of these are the Horton and the variable-source-area (VSA) theories. Horton developed his theory for the infiltration process in the early 1930s. The Horton model (and several later variations) are based on the concept of the soil's surface as a barrier to vertical flow. The VSA theory was presented first by Hewlett (1961) and by Hewlett and Hibbert (1967) in response to phenomena unexplained by traditional hydrologic theories.

7.2 Model Comparisons

MEPAS, MMSOILS, and PRESTO-EPA-CPG each take slightly different approaches to simulating overland flow and the surface water pathway. However, their difference may not significantly affect constituent concentrations at points-of-concern. Each model incorporates a surface contaminant source term, a runoff model, an erosion model, and a surface water mixing component. Table 7.1 compares the capability of the models.

7.2.1 Rainfall-runoff

A significant percentage of the water associated with rainfall-runoff is present in the subsurface flow system before a storm begins (antecedent moisture). In addition, simple hydrologic abstractions based upon conditions at the soil surface cannot predict these contributions, nor their origin within a watershed, even though proper application of these techniques will quantify rainfall-runoff accurately. The complexity of the rainfall-runoff process, the importance of surface-subsurface interactions, and the modeling of surface water flow pathways are not fully implemented into MEPAS. MMSOILS, or PRESTO-EPA-CPG; no subsurface contributions to surface water bodies are implemented into their rainfall-runoff components. Subsurface contributions to surface water bodies are computed solely by the ground water submodel. PRESTO-EPA-CPG uses a physically-based approach to estimate runoff by evaluating the vertical movement of water in the vadose zone beneath the site. Modifying this procedure to evaluate vadose and water table conditions throughout the catchment would generate runoff computations consistent with VSA theory. However, MMSOILS and MEPAS (both of which are based upon an Hortonian approach to the rainfall-runoff process) cannot simulate rainfall-runoff flow pathways.

Table 7.1 Surface water pathway: Comparison of capabilities.				
	MEPAS	MMSOILS	PRESTO-EPA-CPG	
Runoff Calculations	SCS-CN1	SCS-CN'	Physically Based Deterministic Approach	
Erosion	MUSLE⁴	USLE ²	USLE ²³	
Transport				
Miscible	yes	yes	yes	
Adsorbed on Soil	yes	yes	no	
Stream Mixing	coupled, 2D, steady-state advection-dispersion	uncoupled, 1D complete mix	uncoupled 2D, steady-state advection-dispersion	

1. Soil Conservation Service Curve Number method

2. Universal Soil Loss Equation

3. Eroded material is removed from the model and not transported off-site

4. MEPAS uses the Modified USLE - MUSLE (Onstad and Foster 1975; Onstad et al., 1976; Mitchell and Bubenzer, 1980; Novotny and Chesters, 1981)

yes or note = option is available

no = option is not available

The U.S. Soil Conservation Service Curve Number (SCS-CN) method (a variant of the Horton method) is used to compute runoff in the MMSOILS and MEPAS models. This empirically-based procedure was designed to be used on a storm-by-storm basis. The SCS-CN method employs a series of curves that relate runoff volume (Q) to precipitation (P) and watershed storage (S):

$$Q = (P - 0.2S)^2$$

P + 0.8S

This approach is used widely, and accurately predicts runoff volumes on the scale of a watershed. MMSOILS modified the interpretation of a storm in implementing the SCS-CN procedure. The total monthly depth of precipitation is broken into individual storms of equal magnitude by dividing the monthly value by the total number of days per month with precipitation. The antecedent moisture conditions are estimated from the number of days it rained in a particular month. The authors of MMSOILS recognized that these assumptions would give an approximation of runoff volumes using the SCS-CN method, but that this procedure was consistent with the available data.

The rainfall-runoff component in MEPAS uses the same procedure and is based upon the same assumptions as made in MMSOILS. In the rainfall-runoff module in PRESTO-EPA-CPG, overland flow is modeled using a modification of the onedimensional momentum and continuity equations, and infiltration rates are based upon subsurface conditions. The equation for surface water, soil moisture, and evaporation each is solved on the time-scale of minutes and hours over the course of an individual However, a peer review subcommittee (USEPA, 1984) that evaluated the storm. rainfall-runoff sub model of PRESTO-EPA-CPG was concerned that: "...(i) the rate of infiltration is insensitive to variation in the slope of the trench cap; and (ii) the results are highly dependent on the initial water storage value which can not be initialized by the user." Hydrologists have recognized for a long time that these two factors are important for estimating runoff. Nevertheless, since the solution of the equations employed by PRESTO-EPA-CPG is an initial value problem, the error in the assumed initial value can be eliminated by ignoring the initial period of analysis. Based on the extensive trial runs that EPA performed, the maximum length of simulation has never exceeded 5 years, and normally was 3 years, before the initial water storage value reaches equilibrium. Since the PRESTO-EPA-CPG model has had this adjustment to the initial water-storage value built-in to the model, the difficulty of initializing the storage value is virtually solved. As to the insensitivity of the rate of infiltration to the slope of trench cap, this is caused by the relatively large numerical error. This error can be suppressed by selecting smaller space and time steps.

Input Data requirements for the three models are summarized in Table 7.2. PRESTO-EPA-CPG has extensive requirements for climatological data, and hourly precipitation data are required for each day of the year to run this model. Rainfall-runoff and the associated erosion and transport of contamination are short-term transient phenomena controlled by individual storms. A single, short-duration high-intensity thunderstorm will cause more erosion and transport of constituents than a long-duration, low-intensity storm of equal volume. Detailed climatological data are required to simulate these processes.

7.2.2 Erosion and transport components

All three models use the universal soil loss equation (USLE) to approximate soil erosion across the site (Wischmeier and Smith, 1978). This equation is based on a number of empirical relationships (factors) that followed from the analysis of years of accumulated rainfall and erosion data. The equation that embodies this approach is:

$A = R \bullet K \bullet SL \bullet V \bullet P$

where the average soil loss (A) is the product of the rainfall (R). soil erodibility (K), slope (SL), vegetation (V), and management/conservation practice (P) factors. Representative values for these factors for areas within the 48 contiguous states are given in Wischmeier and Smith (1978).

MEPAS uses a modified form of the USLE (MUSLE) recommended by Foster (1976) for use at sites where storm events are to be analyzed. In MMSOILS and These two models have MEPAS contaminant transport is linked with erosion. components that simulate constituents in the runoff which are in solution and sorbed onto the soil being eroded off the site. PRESTO-EPA-CPG accounts for the erosion of the cap at a site, but does not transport the eroded material and associated contaminants; it is simply removed from the system. This is because the standardized PRESTO-EPA-CPG model assumes that the material used for trench-cap construction is clean soil. The eroded soil would not contain contaminants as long as the protective cover is functioning effectively. However, when the protective cover is totally eroded away, the soil would begin to contain contaminants. However, PRESTO-EPA-CPG simulates the transport of dissolved constituents in surface runoff. Contaminants adsorbed onto soils exposed to precipitation and runoff are partitioned off, and considered to be in equilibrium with constituent concentrations in the water. These transport components in each of the models represent distributed source terms (nonpoint sources) to down-slope surface water bodies.

7.2.3 Surface water mixing

MEPAS, MMSOILS, and PRESTO-EPA-CPG use a similar approach to assess radionuclide impacts within surface water bodies. Constituents may be delivered via the rainfall-runoff process, seepage through the movement of ground water, or as direct discharge from the waste site. MEPAS uses a plug-flow-with-dispersion approach for the surface waterborne component (Whelan et al., 1987). MMSOILS uses a simple, complete-mix model for assessing impacts. MMSOILS includes stream and surface water body (lake or pond) submodels, while MEPAS includes a stream and a wetlands. component. The wetlands component in MEPAS has sufficient flexibility to simulate a surface water body also. The stream component is a one-dimensional approximation in MMSOILS, while MEPAS includes a two-dimensional, vertically averaged stream-flow model with unidirectional advection in the flow direction and dispersion in the transverse direction (Whelan et al., 1987). PRESTO-EPA-CPG considers flow within surface water bodies to be one-dimensional. However, transport is evaluated using a two-dimensional (lateral and transverse) steady-state approximation. Additional surface water pathway components can be incorporated also into the PRESTO-EPA-CPG and MMSOILS models because within these two models the surface water components are uncoupled from the other submodels.

Table 7.2 Data input requirements of the surface water pathway.				
	MEPAS	MMSOILS	PRESTO	
Climatological Data		<u> </u>	· · · · · · · · · · · · · · · · · · ·	
Precipitation	Monthly Summary	Monthly Summary	Hourly Data	
Storms	Index on storm type	Average Number of Storms/Month		
Site Parameters				
Vegetative Cover	yes	yes	yes	
Land surface Slope	yes	yes	yes	
Antecedent Moisture	SCS curve number	Estimated from storm frequency	Computed from soil conditions in the vadose zone	
Waste Concentrations	yes	yes	yes	
Soil Parameters		• <u> </u>	· · · · · · · · · · · · · · · · · · ·	
Bulk density	yes	yes	yes	
Porosity	Calculated from specific weight and bulk density	yes	yes	

7.3 Developer Updates - Surface Water Pathway

7.3.1 MEPAS

Droppo (1994) reports that efforts are underway to add to MEPAS specific environmental transport capabilities for wetlands, lakes, estuaries, and river sediment interactions.

7.3.2 PRESTO-EPA-CPG

The modified version of the PRESTO-EPA-CPG model (designed for cleanup scenarios) will be able to simulate contaminants in the surface runoff from the beginning of a simulation, if the scenario of contaminated soil without soil cover is selected.

8. FOOD CHAIN MODELING

8.1 Introduction

Food chains are biospheric pathways through which humans are exposed to environmental contaminants. They are represented by bioaccumulations of contaminants in the edible portions of animals and plants that are affected by the facility. Food chains consist of one or more trophic levels (steps) between the physical environment and human intake of contaminants (Figure 8.1).



Figure 8.1. Basic food chains as depicted in risk assessments.

8.2 Comparisons of Models

Food chains are described as part of the exposure-dose models in documentation for MEPAS (Whelan, 1993), separately in MMSOILS (USEPA, 1992). and as agricultural data supporting exposure estimates in PRESTO-EPA-CPG (USEPA, 1987). MEPAS documentation has detailed formulas to describe each aspect of food chain modeling. As part of its equations for animal feeds, leafy vegetables, and other produce, MEPAS separates descriptions by the origin of plant contamination from wet or dry atmospheric deposition, irrigation, or accumulations in soil. Both foliar and root uptake are described. Table 8.1 summarizes the descriptions of the food chain in the models, and Table 8.2 gives more detailed descriptions of each level in the food chain.

MEPAS, MMSOILS, and PRESTO-EPA-CPG use inputs of time-weighted average concentrations of contaminants. Equations are given for estimating the average concentrations of contaminants at the location of exposure resulting from transport in media and food chains. Measured concentrations can be used instead of those calculated in MEPAS.

Table 8.1 Summary of food chain features in models.			
	MEPAS	MMSOILS	PRESTO-EPA-CPG
Selection of Contaminant			
Hazardous Chemical Waste	yes	yes	no
Radioactive Waste	yes	no	yes
Transfer to Plants			
From Air	yes	yes	yes
From Irrigation	yes	yes	yes
From Soil	yes	yes	yes
Transfer to Animal Products		yes'	J
Meat and Milk	yes	yes	yes
From Air Deposition on Feed Crops	yes	yes	yes
From Irrigation of Feed Crops	yes 🛛	yes	yes
From Soil Consumption	no	yes	yes⁴
From Drinking Water	yes	yes	yes
Finfish	yes	yes'	yes⁴
Shellfish	yes	no	no

1. Combines intake from forage, soil and water.

2. Includes pasture grass, stored feed and leafy vegetables.

3. Calculations based on either water or sediment concentrations.

4. Included in the modified model adaptable to cleanup scenarios.

The irrigation pathway to food chain transport is not well described in MMSOILS, and uptake into plants does not account for edible fractions. For vegetation, MMSOILS uses a general food chain equation to describe atmospheric deposition and bioconcentration from contaminated soil, with a specific description in root crops of the bioconcentration of contaminants from soil. For plant materials, the use of measured concentrations in the three models negates the need for such distinctions. MEPAS and PRESTO-EPA-CPG distinguish leafy vegetables from other types of produce. The number of days in a growing season that vegetable matter including pasture grass and feed is exposed to radionuclides and the fraction of animal feed that is contaminated is considered in PRESTO-EPA-CPG estimates. MEPAS includes the length of the growing season in vegetable and feed-crop production also. All feed for milk cows is assumed to be contaminated forage. All feed for meat animals is assumed to be grain-type plants. If some of the feed is uncontaminated, then the user may modify the intake rates of animal feed to reflect the proportion of contaminated intake.

Table 8.2 Details of food chain levels in the models.					
	MEPAS	MMSOILS	PRESTO-EPA-CPG		
Plant	Feed crops for	Pasture grass and hay	Grass		
	animals	Above around			
	Leafy vegetables	includes leafy (lettuce), and	Leafy vegetation		
	such as lettuce,	silage (com), exposed			
	cabbage, and spinach	produce (non citrus fruits,	Produce		
ļ		berries, field crops —	including grains and root crops		
	Other vegetables	cucumber, tomato,			
	including grains, root	squash, eggplant)			
	crops, and food not				
	generally exposed to	Below around			
	depositional material	root crops			
Meat	beef	beef	beef		
	pork		goat		
	bovine, poultry		······		
Milk and	cow	cow	cow		
Milk Products			goat		
Fish	freshwater finfish and shellfish	freshwater finfish	freshwater finfish and shellfish		

A single formula in MMSOILS describes transfers to animal products (meat and milk) by combining the chemical concentrations in, and the intake rates of, animal feeds, soil, and drinking water. The transfer factors in MMSOILS either take into account the fraction of food that is fat and bioconcentration in the organism, or use partition coefficients for transfers from soil to meat and/or to milk. In MEPAS, transfers to animal products account for direct transfers from media, and transfers from media to forage plants and feed. At present, MMSOILS does and MEPAS does not describe transfers to animal products from accumulations in ingested soil, but MEPAS includes animal ingestion of contaminated water. PRESTO-EPA-CPG includes atmospheric, irrigation, and drinking water sources of contamination of vegetation and animal products.

Whole-body concentrations of chemical and radiological contaminants are considered in both finfish and shellfish by MEPAS and PRESTO. MMSOILS describes only chemical concentrations in "fish" (assumed from the documentation to be finfish), but can base its calculations on concentrations in water and/or sediments. Bio-concentration factors can be selected for fish in general, or for particular species. The bioconcentration factors for contaminants in the water column are adjustable also for the lipid content (%) of fish. MMSOILS uses a sediment-to-fish partition coefficient for chemicals in sediments. MEPAS does not relate concentrations in aquatic animals to those in the sediments.

8.3 Developer Updates Food Chain

None of the models plan future updates that would have any direct impact on assessing transport and exposure via the food chain.

9. EXPOSURE ASSESSMENT

9.1 Introduction

Often, exposures and doses are confused. Exposures are quantities of toxic or carcinogenic agents that are potentially taken into the human body, or (as described by Ruttenber, 1993a,b) "...the contact between an organism and its environment". Exposures (e.g., mg, g, pCi) to a contaminant are estimated usually by multiplying the intakes of environmental media or foods (e.g., L, m³, kg) by the respective concentrations of the agent in the media and/or foods (e.g., mg per L, g per m³, pCi per kg) and summing their products. Exposure rates include specified periods, such as mg per d or pCi per yr. Exposures to chemicals are generally expressed in metric units of mass, while exposures to radionuclides are expressed in standard units of picocuries (pCi) or in *System Internationale* (SI) units of Becquerels (Bq).

Exposure pathways are the last stage of transport modeling, and include those parts of the transport directly related to the behavior and characteristics of those at risk. Exposure estimates are affected by uncertainties in pathway exposure factors (PEFs - McKone, 1990). PEFs are terms that translate unit concentrations in media (e.g., pCi per L) and food chain components into exposures per unit time (exposure rates). PEFs use information on human physiology and behavior, and environmental transport for specific media (McKone, 1990). These uncertainties arise from biological and behavioral variations, as well as the accuracy and precision of the estimated values for each parameter. Many characteristics important to personal exposure are constant, or have a near-constant distribution nationwide (e.g., breathing rates). Others (such as intake of local foods) can be significantly different, depending on local production and exports.

9.2 Comparison of Models

The scope and complexity of the food chain and exposure calculations for multimedia pathways vary with each of the three models. MEPAS covers a wide variety of sources of movement in the food chain and human exposure to chemical and radioactive contaminants (Table 9.1). This coverage includes on-site and off-site pathways. MMSOILS analyzes on- and off-site exposures to chemicals buried in the soil. PRESTO-EPA-CPG analyzes on-site and off-site food chain transport and human exposures for buried, low-level radioactive wastes.

MEPAS, MMSOILS, and PRESTO-EPA-CPG use inputs of time-weighted average concentrations of contaminants. The exposure modules provide users with equations for estimating the average concentrations of contaminants at the location of exposure resulting from transport in media and food chains. Measured concentrations can be used instead of those that are calculated in MEPAS and PRESTO-EPA-CPG, but not in MMSOILS.

Table 9.1 Summary of exposure features in models.			
	MEPAS	MMSOILS	PRESTO-EPA-CPG
Contaminant Selection			
Hazardous Chemical Waste	yes	yes	no
Radioactive Waste	yes	no	yes
Intakes from Ingestion of			
Drinking Water	yes	yes	yes
Shower Water	yes	no	no
Swimming Water	yes	no	no
Leafy Vegetables	yes ²	yes	yes
Other Produce	yes ¹²	yes ⁵	yes
Meat	yes	yes	yes
Milk	yes	yes	yes
Finfish	yes	yes	yes
Shellfish	yes	no	yes
Special Food	yes	no	eggs
)
Shoreline Sediment	yes	no	yes
Soil	yes'	yes	yes⁴
Intakes from Inhalation			
While Showering	yes	no	no
Of Air	yes	yes	yes
Of Re-suspended Soil	yes	yes	yes
Intakes from Contact	· ·		
While Showering	yes	yes	no
While Swimming	yes	yes	no
With Shoreline Sediment	yes	no	no
With Soil	yes	yes	no
With Volatiles in Air	yes	no	no
External Exposures from Radiation: while	yes	no	air immersion, ground
Swimming and Boating; in air; Soil and			surface
Shoreline Sediment; or from			Í
Measurements of Direct Radiation.			

1. From air deposition on crops.

2. From irrigation of crops.

3. Estimations based on either measured concentrations or on calculated accumulations in soil after atmospheric deposition.

4. Included in the modified model adaptable to cleanup scenarios.

5. Root crops.

MEPAS and MMSOILS (as described below) incorporate exposure rates in their formulas for doses from chemical contaminants. Both MEPAS and PRESTO-EPA-CPG use additional special algorithms for ¹⁴C and ³H in vegetable and animal product analysis (see Chapter 10).

Although MEPAS and MMSOILS describe human exposures from ingesting water during swimming, only MEPAS describes ingestion during showering. In MEPAS, exposure rates for ingestion of contaminants in vegetable matter, in animal products, and in special foods are described separately for each transport medium.

MEPAS separately calculates the rates of ingestion of contaminants in shoreline sediments and the soil contaminants. Soil contaminants can be described either by measured concentrations, or by calculated accumulations from atmospheric deposition. Similarly, uptakes from contact with shower water, swimming, shoreline sediments, and soils are described separately.

MEPAS calculates exposure rates separately for inhaling contaminants in air, showers, and re-suspended soil. Also, it is the only one of the three models that distinguishes indoor from outdoor inhalation, which is an important procedure in estimating exposures to volatile organic chemicals and radon.

For radioactive materials, MEPAS models external exposure from irradiation by radionuclides in air, soil, shoreline sediments, and from radionuclides in water during swimming, and boating. Measurements of direct radiation can be used in the exposure calculations also.

In MMSOILS, exposures to non-carcinogenic toxic chemicals are compared to available Reference Dose (RfD) or Health Advisory (HA) values for comparable intervals. Average daily intake rates (mg per kg per d) are time-weighted for 1 day, 10 days, longer periods, and for sub-chronic and chronic periods. HA values (exposure rates in mg per day) are modified to RfD units (dose rates) by adjusting for body weight.

For radionuclide exposures, PRESTO-EPA-CPG estimates include the period of the growing season that vegetable matter is exposed, and fractions of human intake of water and animal products that are contaminated. Animal products are distinguished as meat and milk from cattle and/or goats.

9.3 Developer Updates - Exposure Assessment

Future versions of MEPAS will include ingrowth of progeny in the exposure assessment component of the model (Whelan, personal communication, 1994). No updates are planned for MMSOILS and PRESTO-EPA-CPG that would have a direct impact on the calculation of exposures for any of these models.

10. DOSIMETRY/RISK ASSESSMENT

10.1 Introduction

Dose-assessment codes integrate two components into the assessment of risk: one component calculates the transport mechanism of the released contaminant, and the other calculates the human uptake and dose associated with the exposure. This chapter explores how MEPAS, MMSOILS, and PRESTO-EPA-CPG translate exposures from various sources into numerical estimates of dose and risk (e.g., the number of excess fatal cancers). The estimation of radiation dose is discussed in some detail below because dose estimation for radioisotopes must be treated differently than that for chemicals.

In contrast to chemicals, the effect of radioactive contaminants on humans is a function of the nature of the energy released during their radioactive decay. Radiation is emitted by a radioisotope when it transforms (disintegrates) into another isotope (e.g., ²²⁶Ra to ²²²Rn). Each radioisotope is unique, and the decay rate, energy, and the type of radiation differ. The term activity expresses the number of disintegrations of a radioisotope per unit time. The fundamental unit of activity was the Curie (Ci, or 3.7 x 10¹⁰ disintegrations per second, equal to the activity of 1 g of ²²⁶Ra), but the current SI unit is the Bq (i.e., 1 disintegration per second). The most common types of ionizing radiation are alpha (a) and beta (B) particles, and gamma (g) rays (photons). Each of these three types can be emitted over a range of energies, expressed commonly in units of thousands of electron volts (KeV), or millions of electron volts (MeV). Each radionuclide has its own characteristic radiation type or types and range of associated energy levels. Alpha particles can travel only about 2 or 3 cm in air and no more than about 0.01 mm in body tissue because they have mass. On the other hand, beta particles can travel much further in air and tissue, yet have about the same kinetic energy. A 1 MeV beta particle can travel approximately a meter in air and can likely penetrate the thickness of human skin, but not much beyond that. The minimum energy required for skin penetration for alpha and beta radiations are 7.5 MeV and 70 KeV, respectively. External alpha radiation is not often of concern for the purpose of radiation protection since few alpha decays achieve energies in that range. On the other hand, a weightless 1 MeV gamma-ray can penetrate a sheet of paper or aluminum foil easily, and could pass entirely through the human body. Therefore, gamma radiation is the principal source of concern for external radiation exposures.

Doses for chemicals are the amounts of toxic or carcinogenic agents (or their metabolically activated products) that reach a tissue or organ within the body. Doses are expressed in mass of agent accumulated per unit mass of organ or body weight. Dose rates include specified periods in the expression (e.g., g per kg per d, pCi per kg per d). Dose estimates are derived generally from exposure estimates by using dose conversion factors, which usually represent the fraction of exposure that is delivered to a target organ (or target organs), with adjustments for temporal factors, retention, and conversions to active progeny. Dose factors have been defined extensively for radionuclides, but there is a great deal of uncertainty for chemical doses. Therefore,

risk factors are expressed often in reference to exposures because it is easier to quantify exposures (e.g., EPA's HEAST and IRIS expressions of risks per unit ingested or inhaled).

Radiation dose has been expressed in units of rads (radiation absorbed dose), and rem (roentgen equivalent, man). The rad is a measure of the energy per unit mass (100 erg/gm) delivered to any mass when a given amount of radiation is absorbed. The rem is a special unit of dose equivalent and depends on the type of radiation absorbed (ICRP, 1990). The dose equivalent rem is numerically equal to the product of an absorbed dose in rads and a quality factor (also termed the radiation weighting factor [ICRP, 1991]). For example, neutrons and alpha particles deliver energy in high density packets, while X- and gamma rays deliver the same amount of energy at lower density. Quality factors for radiation are represented usually by the term relative biological effectiveness (RBE), which is a ratio of the magnitude of a particular biological effect of one type of radiation to the magnitude of the same effect of another type of radiation. The SI units for rad and rem are the Gray (Gy) and Seivert (Sv), respectively. One Gy (1 Joule/kg) is equal to 100 rads, while one Sv is equal to 100 rem.

One of the key parameters in deriving the dose to an individual or population is the dose conversion factor. This factor relates a given intake of radioactive material to a radiation dose. In general, the dose conversion factors are derived from recommendations made by the International Commission on Radiation Protection (ICRP). The ICRP recommendations on dose limits are the primary guidance documents used by international and national organizations for estimating effects of ionizing radiation exposure on radiation workers and members of the public (ICRP, 1977, 1979, 1986, 1988, 1989, 1990). Within the United States, the methodology for dose conversion is based on guidance from five different organizations: the ICRP, the National Council on Radiation Protection and Measurement (NCRP, 1993), DOE (DOE, 1988a, 1988b), EPA (USEPA, 1988a, 1993), and NRC.

10.2 Review of Models

Outlined below are the methods used by PRESTO-EPA-CPG and MEPAS to calculate doses from radiation exposures. MMSOILS does not calculate a radiation-based dose; it provides comprehensive analyses of pathways and receptors for on- and off-site exposure, and it is limited to the transport of non-radiogenic chemical materials. Using MMSOILS to predict radiation dose from exposures requires additional health-physics analyses to convert the intake dose and correct for decay. For this reason, we discuss only chemical and not radiation dose for MMSOILS in the text that follows.

10.2.1 Overall dose

10.2.1.1 Chemical Dose

Intakes of chemicals are referred to as administered doses (AD) to conform with RfD values, and MMSOILS assumes that the absorbed fraction of intake is 100% in humans. ADs are calculated as mg per day for water and food ingestion (vegetable, meat, milk and fish), and inhalation or mg per occurrence for soil ingestion. The AD for soil contact are expressed as mg per visit to the contaminated area, and the calculations may require modifications to adjust for alterations of chemicals during cutaneous transfer. Although MMSOILS does not specify ingestion of, nor contact with, shoreline sediment, it is assumed that these exposures can be described by the comparable equations for soil ingestion and contact

Carcinogenic chemical intakes, as 70-year lifetime average daily doses, are compared to EPA's potency factors (now supplanted by slope factors — USEPA, 1989). There is a marked inconsistency in the use of 75-year lifetimes for toxicity and 70-year lifetimes for carcinogenicity.

10.2.1.2 Radiation Dose

The current version of PRESTO-EPA-CPG employs dose conversion factors developed by Eckerman (USEPA, 1994) to calculate dose from internal and external exposures (Rogers and Hung, 1987). The dose conversion factors are extracted from the RADRISK data file (Dunning et al., 1980) and the weighting factors are consistent with the definitions used in ICRP Publications 26 and 30 (ICRP, 1977 and 1979). The effective dose equivalent is the weighted sum of the 50-year committed dose equivalent to the specified and remainder organs. The cancer risk coefficients are calculated from the radiation risk models based on 1980 U.S. vital statistics. On the other hand, the radionuclide genetic risk coefficients for serious heritable disorders to all generations are calculated from the product of the average absorbed dose to the ovaries and testes up to age 30 per unit intake before that age. Genetic Risk Coefficients of 2.60 x 10^{-2} and 6.9×10^{-2} Gy⁻¹ for low-LET and high-LET radiation are used to calculate the risk conversion factors, respectively (USEPA, 1994b).

PRESTO-EPA-CPG employs the DARTAB submodel to estimate both exposure and annual committed doses (mrem per y) for as many as 40 radionuclides, by adding the weighted doses to each organ from all pathways of exposure. Exposures from ingested intakes of radionuclides are expressed as person pCi per year. External irradiation exposures from air or contaminated ground surfaces are, expressed as person-pCi per m³ (volume), and person-pCi per m² (surface) respectively. DARTAB combines estimates of radionuclide exposure with dosimetric and health effects data to generate predicted impacts.

MEPAS uses the methodology in Federal Guidance Report -11 (FGR-11 [USEPA, 1988]) to calculate dose from internally deposited radionuclides. For external

exposures, MEPAS obtains dose using the Eckerman (USEPA, 1994) dose conversion factors. In contrast to PRESTO-EPA-CPG which calculates and reports a dose. MEPAS calculates dose rate, as rem per unit time, but only reports fatal cancer risks. These risks $(5.0 \times 10^{-2} \text{ fatal cancers Sv}^{-1})$ are consistent with the latest ICRP recommendation (ICRP, Publication 60, 1991) for radiation workers. If MEPAS is used to calculate risk for the whole population, the suggested risk factor is 7.3 x 10^{-2} fatal cancers Sv⁻¹ (NCRP, 1993); i.e., the sum of the fatal cancer, non-fatal cancer, and severe genetic effects. These cancer effects represent a stochastic outcome. MEPAS does not calculate an equivalent dose for any single organ or tissue for evaluating deterministic health effects like those associated with organ-seeking nuclides (e.g., iodine for thyroid, and strontium for bone).

MEPAS and MMSOILS estimate doses (e.g., mg per kg per d; pCi per kg per d) on the basis of average daily exposures. This may not determine risks accurately, for example, when exposures vary widely in intensity and duration. PRESTO-EPA-CPG uses annual exposures because it estimates maximum doses on a year-by-year basis (up to 10,000 years) but, overall, this is similar to the assessment of radionuclides in MEPAS. On the other hand, PRESTO-EPA-POP calculates the fatal cancer and serious genetic risks for the local and downstream basin population. However, the uncertainty of the overall risk assessment tends to increase with time because of the increasing uncertainty of demographic predictions. Since the PRESTO-EPA-CPG model uses a hypothetical scenario in which the critical population resides in a userassigned location and calculates the dose for each person, the uncertainty in the demographic distribution will not be the concern of this analysis. In PRESTO-EPA-POP, the uncertainty in the demographic distribution will affect significantly the uncertainty of the number of the fatal cancer and serious genetic effects - a situation that applies to all models.

10.2.2 Inhalation dose

There is a significant relationship between particle size, lung retention, and dose for estimating dose due to inhalation. The physical association of radioactivity with micron size and sub-micron size particles is crucial for the inhalation pathway. The smaller particles penetrate deeper into the lung, are more efficiently deposited there, and are cleared inefficiently as long as they are insoluble.

All assumptions associated with the intake-dose constants of FGR-11 (USEPA, 1988) become default parameters within MEPAS. MEPAS uses a 1 micron particle size for aerosols based on FGR-11. Furthermore, MEPAS uses the ICRP-30 dynamic lung model and its compartment parameter values, the so-called D-W-Y lung clearance class for chemical transportability (ICRP, 1979). In this case, D refers to those materials that can be removed from the lung in days, W in weeks, and Y in years, respectively. The PRESTO-EPA-CPG organ dose rates are calculated from pre-calculated conversion factors, derived using the default value of 1 micron particle size for aerosols and the lowest solubility D-W-Y lung class (class Y is used in most cases). These default values are recommended by ICRP.

10.2.3 Radon/Thoron progeny and long-lived fission products

The modified PRESTO-EPA-CPG version adaptable to cleanup scenarios includes a radon inhalation pathway. MEPAS does not derive dose calculations for natural radon/thoron progeny (RTP), but allows the user to specify a radon emission rate from which atmospheric transport of radon and progeny is evaluated using "mock radon" radionuclides. This representation allows an evaluation of dose from radon. It includes an equilibrium amount of short-lived progeny and the maximum amount of long-lived progeny, thus providing a conservative estimate of radiation risk. ²²²Rn, and ²²⁰Rn are a concern at sites contaminated with ²²⁶Ra or ²²⁴Ra, respectively. Since many sites have high levels of Ra, failure to account for dose due to ²²²Rn,²²⁰Rn would be a significant deficiency.

Long-lived fission products and nuclear materials cannot be neglected necessarily because of their low specific activity, especially those that have been classified as "most hazardous materials" such as neptunium (Np), plutonium (Pu), and americium (Am). On the other hand, those radioisotopes with short half-lives (e.g., isotopes of Np, Pu, and Am other than ²³⁷Np, ²³⁹Pu, and ²⁴¹Am) are of less concern to any health risk assessment of long-term waste disposal. However, the release of contamination that includes long-lived isotopes like those of ²³⁷Np, ²⁴¹Am, and ²³⁹Pu is of the utmost concern for any environmental safety and health study.

10.2.4 Period of exposure

PRESTO-EPA-CPG model calculates the rate of dose commitment (mrem/yr) by multiplying the exposure rate (pCi/yr) with the dose-conversion coefficient (mrem/pCi). A 50 year dose commitment factor is used for this calculation. The value of the dose commitment factor is obtained from FGR-11 for each radionuclide. MEPAS bases its dose analysis on intake for a user-defined exposure duration (70 year default).

10.2.5 Individual vs. population-based dose

MEPAS calculates the dose to an individual located at some place in time and both individual and population risks. Early versions of MEPAS calculated a Hazard Potential Index (HPI) which is based on the population exposure. Neither the MEPAS or MMSOILS models calculate onsite exposures. The original version of PRESTO-EPA-CPG model calculated the annual and maximum dose to the on-site farmers from drinking, irrigation, and cattle-feed pathways. The estimation of the cumulative fatal and genetic health effects does not include normally the effects to on-site farmers. Since the PRESTO-EPA-CPG model calculates the total population health effects by adding the local population health effects with downstream population health effects, the user may combine the on-site farmers into the local population. The results of analysis include the fatal and genetic effects from the on-site farmer and the downstream population.

10.3 Developer Updates - Dose/Risk Assessment

10.3.1 MEPAS

Planned updates for MEPAS include modules to calculate ecological risk, acute human risk, and worker risk (Droppo, 1994).

MEPAS is being incorporated into the Remedial Action Assessment System (RAAS), a screening tool for cleanup remedies. MEPAS' baseline risk assessment is used by RAAS as a starting point for estimating residual risk to evaluate the effectiveness of alternative remedies.

10.3.2 PRESTO-EPA-CPG

PRESTO-EPA-CPG is being modified to include dose from progeny nuclide ingrowth and for the soil-ingestion pathway (Hung, 1994). Version 2.1 of PRESTO-EPA-CPG contains also revised computational models, procedures, and data for dose conversion to conform with ICRP 30. SI units are adopted also for radioactivity and dose equivalent. The modified PRESTO-EPA-CPG model will improve the on-site residence to cover all applicable scenarios that could be adapted to a cleanup scenario.

11. UNCERTAINTY ANALYSIS

11.1 Introduction

Uncertainties in risk assessment are important in making risk management decisions. In a risk assessment, descriptions of uncertainties may indicate the quality of information, range of knowledge, and level of confidence available. Extensive sensitivity and uncertainty analyses were made to develop EPA's Low-Level Waste Environmental Standards. Several factors contribute to these uncertainties, including: limitations in the data that characterize sites and source terms, uncertainties in scenarios and choices of parameters to fit different scenarios, uncertainties in formulating the transport model and in physical parameters used as input to the models (e.g., diffusion coefficients), exposure parameters, and dose-response relationships. The word parameter is used in this document as a component (= property or variable) that can be characterized either quantitatively or qualitatively. Some factors contributing to the uncertainty in final risk estimates are more important than others.

Uncertainty arises from combinations of heterogeneity (variability), errors in measurement, and lack of knowledge.

- Heterogeneity is the variability within a parameter, such as the variability in the characteristics of a population. For example, it is relatively easy to determine the amount of water that an individual drinks daily, but the amount will vary from day to day and among individuals in a population.
- Error in measurement arises from inadequacy of sampling, sampling biases, errors in the measurements, and imprecision.
- Lack of knowledge can involve parameters that are expressed quantitatively and components of a risk assessment that do not have numerical values. Major sources of uncertainty include inadequate knowledge of physical processes, such as environmental transport mechanisms, and gaps in qualitative knowledge, such as future landuse scenarios. Parameters and their ranges of values can be affected profoundly by choices among these components of a risk assessment, in turn affecting the overall uncertainties of the risk estimates.

Most parameters used in risk assessments contain elements of heterogeneity, errors in measurement, and lack of knowledge. For example, the amount of water that is imbibed daily is heterogeneous across a population, but each sample is subject to errors in measurement and sampling bias.

As part of a risk assessment, uncertainty analyses should be performed to determine which parameters exert a significant influence on the overall risk estimates.

Sensitivity analyses are used to assess which parameters are the most important contributors to the magnitude of an overall risk estimate, and they frequently are undertaken as part of a screening-level assessment. These analyses compare all parameters in an assessment for the overall effects of a specific degree of change (e.g., a 20% variation) in each parameter (Morgan and Henrion, 1990).

Uncertainty analyses estimate the contribution of uncertainty associated with each variable to the overall uncertainly of a risk estimate (Rish, 1988). A sensitivity analysis can be performed as part of an uncertainty analysis to identify the parameters that contribute the most to the variance of the final risk estimates. In other words, the analysis quantifies the sensitivity of uncertainty of a risk estimate to a changed range or assumed type of distribution of a single variable.

11.2 Comparison of Models

The three models use deterministic (single) values for parameters. It is difficult in such deterministic assessments to sort out the contributions of individual parameters to the overall uncertainty of the risk estimates, because the calculations can combine high (90th or 95th percentile) parameter values with lower (50th percentile or average) values (Burmaster and Harris, 1993).

The accuracy of the value of the parameters in all three models is difficult to verify. Although such difficulties are balanced by the user's ability to input alternative values, no specific instructions are provided for performing uncertainty analyses as a way of estimating the adequacy and precision of assumptions. The "Documentation and Users Manual for MMSOILS" (USEPA, 1992) expresses the clearest concern about the overall uncertainty of the risk estimates, and of specific parameters MEPAS and MMSOILS suggest and allow input of site-specific and region-specific data to reduce uncertainty for food chain and exposure parameters, and to provide alternative choices for doing some calculations when the concentrations of contaminants have been measured at specific sites. MEPAS also gives some regional data in its reference tables. MEPAS supplies a report, based on site-specific sensitivity analysis, that gives the user information on sensitive parameters in each of the codes comprising the model (Doctor et al., 1990). A second MEPAS report (Droppo et al., 1990) provides a system-wide uncertainty analysis for representative sites and constituents.

11.3 Developer Updates - Uncertainty Analysis

An operational version of a sensitivity/uncertainty module for MEPAS is being tested at several sites (Droppo. 1994). Besides user-input parameters, a version is planned that will allow sensitivity analysis via Monte-Carlo analysis on the physical, chemical, and toxicity parameters associated with health impacts from the MEPAS database. The addition of the capability to perform uncertainty analysis within the existing PRESTO-EPA-CPG model is planned.

12. PARAMETER ESTIMATION AND DEFAULT VALUES

12.1 Introduction

Inaccurate values for input parameters can be a major source of error in health risk assessments. Input data can be faulty because of poor judgment in estimating the parameter and over-reliance upon default values which may not be applicable to a given scenario. The data from which parameter values were derived may not be relevant to the specific set of conditions to be addressed by the model. The determination of a parameter value itself carries some inherent uncertainty since processes within environmental models have a large natural variability in time and space, and such values are based often on experimental data that refer to only a few discrete points in time and space.

In this chapter, the three models are compared in terms of their data requirements, availability of default values, and guidance to select or estimate parameter values. This chapter assesses also the relative importance of different parameters in the given models, based on information in the manuals and in previous reviews. The parameters of greatest importance are the ones that have the greatest potential impact on the outputs for the particular assessment (i.e., long-term environmental and public health risks for environmental restoration and waste management activities). In this context, four categories of model parameters (e.g., rate, time, and duration of a release, nuclide speciation, source strength, chemical and physical form of the release radionuclides), (ii) environmental transport parameters (e.g., wind speed, precipitation height, porosity, sorption, partition coefficients, soil hydrogeological properties), (iii) bioaccumulation parameters, and (iv) dose and exposure parameters (e.g., living and consumption habits, health standards).

12.2 Comparison of Models

12.2.1 Description of the data input requirements for models and their default values

MEPAS has data on more than 576 chemicals and radionuclides in the chemical and sorption K_d databases. The former includes information on a) physical properties, b) environmental decay, c) environmental transfer. d) radiological dosimetry, and e) chemical toxicity. The sorption K_d database contains a matrix of K_d values for each inorganic and radioactive constituent as a function of pH and content in soil of clay, organic matter, iron, and aluminum. The manual gives instructions on how to select or estimate each of these parameters. MEPAS requires the most input parameters of the three models reviewed here. While this allows more site-specific applications of the model, it increases the effort required for determining the parameters at the same time. MEPAS databases provide some default values. However, its manual gives extensive documentation and guidance that helps users in estimating or selecting values for the input parameters. Also, it includes a range of parameter values.

Sorption K_ds for organic constituents are computed within MEPAS using K_{oc} values, organic matter content, and the soil's proportion of sand, silt, and clay. The inorganic and organic K_d values determined by MEPAS are provided to the user as suggested values for each constituent of the soil layer; as such they are not presented as "correct" values. Rather, they are meant to represent typical values that might be found for the constituents of concern. The user can take the suggested value or replace it with site-specific information.

MMSOILS has a database with chemical, transport, decay, and chemical or radiological dosimetry characteristics for 240 pollutants. The code requires several pathway-specific pieces of information (e.g., atmospheric pathway, surface water pathway, ground water pathway, infiltration leaching and recharge, food chain bioaccumulation pathway). One hundred and seventy-seven input values are required, many of which are provided in tables or suggested in the users manual. The manual gives guidance for selecting or estimating the parameter values, but that guidance is not as detailed as that of MEPAS.

PRESTO-EPA-CPG requires input data on site-specific and radionuclide source terms, hydrogeologic and meteorological conditions, radiological dosimetry, and health effects. The manual describes all the required parameters, but includes default values and/or guidance to select/estimate values for only six of them. Since the model provided input data sets for the humid permeable, the humid impermeable, and the arid permeable sites in the United States, it gives a wide spectrum of sites across the United States. Furthermore, since each of the submodels within PRESTO-EPA-CPG is designed to be as dynamic as possible, most of the required input parameters represent system characteristics and are measurable. That is, the PRESTO-EPA-CPG model uses less dependent variables that should be calculated, in theory, by the model as user-assigned input parameters. Therefore, the model requires less guidance to assign input parameters that would require extensive empirical data bases.

12.2.2 Comparison of values from MMSOILS and MEPAS databases

Table 12.1 compares the values from the databases of MEPAS and MMSOILS for a relatively immobile chemical, arsenic. Table 12.2 shows the same data for benzene, a relatively mobile chemical. PRESTO-EPA-CPG was excluded because (i) it includes only radionuclides, not chemicals, and (ii) the documentation provides only a few default values. These comparison tables provide examples of the range in input parameters that can exist between MEPAS and MMSOILS for two typical contaminants.

12.2.3 Source term parameters

Problems related to quantifying the parameters of the source term include sparse or inaccurate information about identifying the types of wastes present, determining the quantities of waste, and estimating waste distribution. Release and solubility parameters define the mass of leachate to be released to the subsurface from a waste management unit. Some site-specific parameters are difficult to ascertain, yet they can have a significant impact on the results. For example, one such parameter is the rate of suspension of particles caused by vehicles disturbing the site. MEPAS accounts for the silt content of the road, vehicle weight, length, frequency of mechanical disturbances, and other such parameters. Different analysts could choose easily different values of these parameters for the same site.

12.2.4 Environmental transport and decay parameters

An important parameter that defines the distribution of the source term among different media is the K_d . K_d plays an important role in estimating the concentration of leachate between the waste management unit and ground water, and between contaminated soil and runoff. Default K_d values in MEPAS represent typical environments and may be conservative because the smallest value (least adsorption) was included usually in the database when there were several values for a given chemical/soil-type interaction (Strenge, Peterson, and Sager 1989). These values should not be used if there are site-specific data for K_d , nor if inorganic and/or radioactive constituents are mixed with organically complexed wastes. In which case, K_d should be set at zero (Strenge, Peterson, and Sager 1989).

The transfer of a contaminant from the topsoil into the atmosphere is dominated by potential evaporation and transpiration (PET). Determination of PET is critical for predicting the volume of leachate from a waste disposal site. MEPAS uses three methods to estimate PET (i.e., modified Blaney-Criddle, Penman, and Penman with correction factor). Each method is applied at each site. The one estimating the lowest value is used in that site's assessment.

Makhlouf and Kavanaugh (1993) performed sensitivity analysis of MEPAS for precipitation-driven leaching involving a relatively immobile constituent, arsenic and a relatively mobile one, benzene. The contaminants could only migrate by dissolution from the top soil into the aqueous phase, followed by migration with the aqueous phase into the partially saturated zone. The conclusions of this study can be summarized as follows:

- An accurate estimate of the initial mass of each constituent present in topsoil is critical to the ability of MEPAS to predict the duration of a release. Predicted values of Maximum Individual Risks (MIRs) are relatively insensitive to the choice of input parameters for the topsoil when the initial mass inventory is constant.
- The estimated MIRs are sensitive to the infiltration rate because this parameter controls the rate of release from the top soil, as well as the rate of migration through the partially saturated zone.
- The estimated MIRs are sensitive also to the choice of input parameters for the saturated zone (e.g., hydraulic conductivity, effective porosity, and dispersivity).
Although these comments may be correct for a specific problem that is being assessed, they are not universally true. For example, if the problem is temporally far-field, the rate of release has no effect on the results; only a change in the source term inventory affects the results. For a temporally near-field case, the rate of release determines the risk. If the soil type is radically altered, then the risk will be influenced substantially by this change.

Table 12.1 Input Parameters for Arsenic.				
	MEPAS	MMSOILS		
Molecular Weight (g/mol)	75	75		
Vapor Pressure (mm Hg)	0.0	0.0001		
Henry's Law Constant (atm m ³ /mol)	NA	1.E-08		
Solubility In Water (mg/L)	0.0	100000		
Organic Carbon Partition Coefficient (Koc) (mL/g)	NA	NV		
Octanol-Water Partition Coefficient (Kow) (mL/g)	0.0	NV		
Partition Coefficient, Kd, (ml/gm) - at pH=	>9 5-9 <5			
Kd for clay+organics <10% of total soil (mL/g)	0.6 5.86 5.86	3.54		
Kd for clay+organics 10-30% of total soil (mL/g)	2.0 19.4 19.2	3.54		
Kd for clay+organics >30% of total soil (mL/g)	2.0 19.4 21.5	3.54		
Kd for aquifer (<i>mL/g</i>)		3.54		
Environmental Half-Life In Air (days)	NV ¹ , 6.9E+07 ²	NA		
Environmental Half-Life In Water (days)	NV ¹ , 6.9E+07	NA		
Environmental Half-Life In Soil (days)	NV ¹ , 6.9E+07 ²	NA		
Ground Water 1 st Decay (1/yr)	NA	0.0		
Unsaturated Sediments 1 st Order Decay (1/yr)	NA	0.0		
Chemical Decay In The WMU (1/yr)	NA	0.0		
Chemical Decay Constant In Off-Site Field (1/yr)	NA	0.0		
1 ^{sr} Order Decay In Stream (1/yr)	NA	0.0		
Fish Bio-Accumulation Factor (1/kg)	100 ¹ , 1.0 ²	NA		
Bio-concentration In Fish (mg/kg fish)/(mg/L water)	NA	1.00		
Sediment/fish Partition Coef. (mg/kg fish)/(mg/ kg soil)	NA	0.00		
Shellfish Bio-Accumulation Factor (1/kg)	40	NA		
Soil-To-Plant Uptake	0.0015 0.01	NA		
Soil-To-Meat Partition Coef. (mg/kg beef)/(mg/kg soil)	NA	0.00		
Feed-To-Meat Coefficient (d/kg)	0.002	NA		
Feed-to-Cow Milk Coefficient (g/L)	0.002	NA		
Transfer Factor For Cattle (kg/kg)	NA	0.002		
Transfer Factor For Milk (mg/kg milk)/(mg/kg intake)	NA	0.00006		
Soil To Milk Partition Coef. (mg/kg milk)/(mg/kg soil)	NA	0.00		
Uptake From Soil To Plant (mg/kg plant)/(mg/kg soil)	NA	0.04		
Soil Moist. To Root Factor (mg/kg root)/(mg//kg solute)	NA	0.00		
Water Purification Factor	0.7	NA		
Deposition Velocity (m/s)	0.001	NA		
Atmospheric Deposition Class	1	NA		
Inhalation Cancer Potency Factor (kg-d/mg)	5.0E+01	NA		
Ingestion Cancer Potency Factor (d/mg)	1.5	NA		

NV = no value is listed in electronic database NA = not applicable

1. = value in electronic database of MEPAS version 3.x

^{2. =} value in manual (Chemical Databases; Strenge, Peterson, and Sager, 1989). Note that the values in subsequent versions of the manual are continuously updated to conform with the values in the electronic database.

Table 12.2 Input Parameters for Benzene.			
	MEPAS	MMSOILS	
Molecular Weight (g/mol)	78	78.11	
Vapor Pressure (mm Hg)	95	94.2	
Henry's Law Constant (atm m ³ /mol)	5.6E-03	5.7E-03	
Solubility In Water (mg/L)	1750	1690	
Organic Carbon Partition Coefficient (Koc) (mL/g)	83	31	
Octanol-Water Partition Coefficient (Kow) (mL/g)	1.32	NA	
Partition Coefficient (Kd) For Waste - at pH=	computed		
Kd for clay+organics <10% of total soil (mL/g)		0.0	
Kd for clay+organics 10-30% of total soil (mL/g)		0.0	
Kd for clay+organics >30% of total soil (mL/g)		0.0	
Kd for aquifer (mL/g)		0.0	
Environmental Half-Life In Air (days)	NV ¹ , 6.9E+07 ²	NA	
Environmental Half-Life In Water (days)	NV ¹ , 6.9E+07	NA	
Environmental Half-Life In Soil (days)	NV ¹ , 6.9E+07	NA	
Ground Water 1 st decay (1/yr)	NA	0.0	
Unsaturated Sediments 1 st Order Decay (1/yr)	NA	0.0	
Chemical Decay In The WMU (1/yr)	NA	0.0	
Chemical Decay Constant In Off-Site Field (1/yr)	NA	0.0	
1 st Order Decay In Stream (1/yr)	NA	0.0	
Finfish Bio-Accumulation Factor (1/kg)	0', 24 ²	NA	
Bio-Concentration In Fish (mg/kg fish)/(mg/L water)	NA	24.48	
Shellfish Bio-Accumulation Factor (1/kg)	0',3.9*	NA	
Sediment/Fish Partition Coef. (mg/kg fish)/(mg/ kg soil)	NA	0.00	
Soil-To-Edible Plant	0', 0.58	NA	
Soil-To-Meat Partition Coef. (mg/kg beef)/(mg/kg soil)	NA	0.00	
Beef Uptake (d/kg)	0',3.36E-06		
Feed-To-Cow Milk Coefficient (g/L)	0.002	NA	
Feed-To-Meat Coefficient (d/kg)	0.002	NA	
Milk Update (d/L)	1.05E-06	NA	
Transfer Factor For Cattle (kg/kg)	NA	0.002	
Transfer Factor For Milk (mg/kg milk)/(mg/kg intake)	NA	0.00000107	
Soil To Milk Partition Coef. (mg/kg milk)/(mg/kg soil)	NA	0.0000000	
Uptake From Soil To Plant (mg/kg plant)/(mg/kg soil)	NA	14.5606	
Soil Moist. To Root Factor (mg/kg root)/(mg//kg solute)	NA	2.12987	
Water Purification Factor	1.00	NA	
Deposition Velocity (m/s)	1.2E-06	NV	
Atmospheric Deposition	1	NV	
Inhalation Cancer Potency Factor (kg-d/mg)	2.9E-02	NV	
Ingestion Cancer Potency Factor (d/mg)	2.9E-02	NV	

NV^T = no value is listed in electronic database NA = not applicable

 = value in electronic database of MEPAS version 3.x
= value in manual (Chemical Databases; Strenge, Peterson, and Sager, 1989). Note that the values in subsequent versions of the manual are continuously updated to conform with the values in the electronic database.

12.2.5 Parameters for bioaccumulation

MEPAS lists some different values of bioaccumulation in its electronic and paper database. For example, benzene's feed-to-meat coefficient has a zero value in the electronic database, and 3.36E-06 value in the paper database. The model user needs to be aware that MEPAS' electronic database is constantly being updated, and the paper database serves only as an example of representative values. In addition, the electronic database of MEPAS contains zero values for those parameters (e.g., finfish bioaccumulation parameter) that are evaluated at run time by MEPAS' exposure assessment component using correlation relationships. Correlation analysis is not used for non-zero values in the database.

12.2.6 Parameters of dose and exposure

When source terms and estimates of contaminant flux along different exposure pathways are determined, the next set of data required includes the more site-specific parameters that determine exposure and dose.

In MMSOILS, the "action levels" for air-borne releases of several contaminants are incorrect. For example, the action level for 1,1,2 trichloroethane is listed as 0.6 μ g/m³, whereas the PEL (Permissible Exposure Level, based on 40 hour work-week) is 45 mg/m³. The action level for selenium is listed as 3.5 μ g/m³, whereas the PEL for selenium is 0.2 mg/m³. A default value of 99.9 mg/m³ is assigned to several other chemicals (e.g., mercury, acetone, dioxane), while their PELs range from 0.1-2400 mg/m³.

In addition, MEPAS Version 3.0 allows the user to input certain uptake and exposure parameters. Documentation is provided for the inclusion of such parameters. There are procedures for modifying MEPAS default parameter files contained in files that can be edited, rather than the previously hard-wired versions.

12.3 Developer Updates - Default Parameters

The number of contaminants in the MEPAS database is under expansion to include new parent radionuclides, and organic and inorganic chemicals (Droppo, 1994). Radioactive decay chains are being expanded also. Whereas the current MEPAS contains approximately 500 chemicals, the September 1994 release contains approximately 700.

13. DISCUSSION/CONCLUSIONS

13.1 Source Term

Hazardous waste sites may leak contaminants into the environment and pose a threat to human health. At many sites, in addition to the general characteristics of the site, the only fact that is known is that hazardous materials are being released. The specific cause of the release of contaminants from that site source may be undefined. In addition, the strength and nature of hazardous releases may vary with time, and the impact may shift among the pathways affected by those releases. These uncertainties challenge the multimedia modeler to arrive at some reasonable approximation for a source term that will simulate closely the actual site release of hazardous waste.

The three models can simulate a variety of source terms; MEPAS has the most varied capabilities for source term modeling of the three models reviewed. None of the models can deal with the presence of free or residually-saturated, non-aqueous liquid, within the source term. Each model bases leachate production on either a steady-state value or on leachate solubility or equilibrium-partitioning.

13.2 Air Transport

Volatile hazardous waste components leaving a site through the atmospheric pathway are subject to the vagaries of weather at the surface of the earth. Air-transport modeling assumes commonly that transport through the atmosphere occurs as a more or less weakly organized plume whose direction, dimensions, and contaminant concentrations are controlled by the speed and direction of the wind, the rate and quantity of precipitation, and the extent of fallout from that plume.

All three models use a standard, sector-averaged, Gaussian-plume approach for air-transport and model annual-average concentrations and exposures. MEPAS and MMSOILS use the same volatilization algorithm. Only PRESTO-EPA-CPG models radioactive decay. Only MEPAS can model atmospheric calm conditions with accompanying channeling and complex terrain characteristics.

13.3 Ground Water Transport

The movement of ground water is most often very slow, and that movement occurs over an area and volume that is often much larger than the area and volume of the source. Once in the ground water, contaminants are isolated and difficult to remove. As an essential human nutrient, almost every human being is exposed in some way to contaminants that originate in ground water, some people much more than others. All of these factors imply that the ground water pathway can pose a serious threat to public health at hazardous waste sites. Therefore, perhaps the most serious limitation of screening-type models like MEPAS, MMSOILS and PRESTO-EPA-CPG is the relative simplicity of their ground water transport components. While each model includes a ground water component that is capable of modeling both unsaturated and saturated transport, that component is simulated using classical assumptions - uniform, linear flow in a homogeneous, layered medium with equilibrium, and reversible adsorption of miscible contaminants. The transport of materials through the ground water system is complex, both in terms of the effect of non-uniform flow regimes and because of chemical reactions between ground water and matrix. The properties of radioactive materials themselves pose special problems. Only MEPAS and PRESTO-EPA-CPG consider the fate and transport of radioactive progeny: although both assume the same adsorption characteristics for progeny as for parent. MMSOILS does not model the decay of adsorbed contaminants.

13.4 Erosion, Overland Flow, Runoff and Surface Water Transport

Multimedia models are very often employed for use at sites where radioactive contamination originates at or near the land's surface. Therefore, source materials may be not only subject to atmospheric conditions or leached into the ground water, but also possibly removed by surface transport processes.

As with the ground water component, MEPAS, MMSOILS and PRESTO-EPA-CPG employ similar, simplistic models for runoff, erosion, and mixing within surface water bodies. These simplistic approaches are based, for the most part, on empirical equations that may have little or no physical basis. The same limitations for simulating the transport of radionuclides that exist for simple ground water models pertain to simple surface water models: accurate flow paths can be very important when modeling constituents that decay, and simple equilibrium partitioning between dissolved contaminants and sediments within surface water bodies may not be sufficient in environments where, for example, resuspension can be important. None of these models considers volatilization from surface water bodies into the atmosphere. MEPAS and MMSOILS have separate subroutines for modeling transport within wetlands and lakes, respectively.

13.5 Food Chain Modeling and Exposure Assessment

The assessment of human health risk is the primary objective of most transport and exposure assessment modeling. The penultimate step before the final calculation of human exposure and risk is to estimate the concentration of contaminants in food and drink to which humans will be exposed. MEPAS includes food chains as an integral part of its exposure-dose component. Food chains are considered separately in MMSOILS and in PRESTO-EPA-CPG as agricultural data supporting exposure estimates. Although MEPAS can be used to model acute toxic atmospheric releases, all three models were designed primarily to handle long-term, chronic exposures. Each of the three models employ comparable, standard methods for estimating exposure to environmental contaminants through the food chain and other pathways. Therefore, the same limitations that exist for all exposure and risk assessments exist for these models. For example, food intake is subject to behavioral variations. Both the quantity and type of foods eaten vary from location to location. In addition, the poor state of knowledge of the combined effects of radionuclides and toxic chemicals may have additional implications for the accuracy of exposure calculations at mixed-waste sites.

13.6 Dosimetry/Risk Assessment

Human health risk is a function of the actual impact that an environmental contaminant has on an individual or group. The quantity of a toxic substance that produces an adverse response in an organism is known as a dose. Dose can refer to individual organs or a whole body; it can be either internal or external; and it can be either acute or chronic. In addition, the model may be designed to calculate either individual or population dose on and/or off a contaminated site.

Only MEPAS and PRESTO-EPA-CPG can calculate human dose from radionuclides. MMSOILS is designed to consider only toxic chemicals. Both MEPAS and PRESTO-EPA-CPG use methods defined by Eckerman to calculate external dose. The chronic dose calculated by MEPAS is based on a default lifetime exposure of 70 years, while PRESTO-EPA-CPG uses 50 years for its dose period. MEPAS calculates individual dose and individual and population risk. Both MEPAS and MMSOILS were designed for the estimation of off-site exposures and dose, while PRESTO-EPA-CPG can calculate both on- and off-site dose by including the on-site population as part of the "local" population.

13.7 Uncertainty Analysis

The accuracy of a predicted outcome cannot be better than the accuracy of the data input to the model. In addition, no matter how accurate the input data is, if the algorithms used by the model do not closely mirror "real-world" processes, the output generated by the simulation will be of little use. Not all input data and not every model algorithm affect the accuracy of the outcome of the simulation equally. Uncertainty and sensitivity analyses are procedures that the model user can follow in an attempt to quantify the impact of parameter (input) and/or structural (algorithm) error.

Uncertainty analyses can and should be performed with any model as long as the user can vary input parameters and observe the results of the simulation. The capabilities for performing uncertainty analyses with the three models reviewed in this report are a function of the number and diversity of input parameters. In this way, PRESTO-EPA-CPG has fewer environmental input parameters than either MEPAS or MMSOILS. MEPAS and MMSOILS discuss methods for estimating more accurate values for site-specific parameters when site-monitoring data are available.

13.8 Parameter Estimation and Default Values

The three models use deterministic (single) values for parameters. It is difficult in such deterministic assessments to sort out the contributions of individual parameters to the overall uncertainty of the risk estimates, because the calculations can combine high (90th or 95th percentile) parameter values with lower (50th percentile or average) values. The accuracy of the value of the parameters in all three models is difficult to verify. Although such difficulties are balanced by the user's ability to input alternative values, no specific instructions are provided for performing uncertainty analyses as a way of estimating the adequacy and precision of assumptions.

13.9 Overall Summary

Table 13.1 presents a summary of the features contained within each of the three models. For the purpose of simulating the transport, fate and effects of radioactive contaminants through more than one pathway, both MEPAS and PRESTO-EPA-CPG are adequate for screening studies; MMSOILS only handles nonradioactive substances and must be modified before it can be used in these same applications. Of the three models, MEPAS is the most versatile, especially if the user needs to model the transport. fate and effects of hazardous and radioactive contaminants.

Table 13.1 Summary of model features.					
	MEPAS	MMSOILS	PRESTO-EPA-CPG		
Contaminant Selection					
Hazardous chemical waste	yes	yes	no		
Radioactive waste	yes	no	yes		
Air Pathway			······································		
Gas/Vapor emissions	yes	yes	yes		
Particulate emissions	ves	ves	ves		
Point/Area/Air sources	yes/yes/yes	no/yes/no	yes/yes/no		
Volatilization	yes	yes	no		
Plume rise	yes	no	no		
Plume reflections on					
ground/lid	yes	no	yes		
Calm conditions	yes	no	no		
Complex terrain	yes	no	no		
Ground roughness	yes	no ⁷	yes		
Dry deposition	yes	yes	yes		
Wet deposition	yes	no	no		
Radioactive decay	yes	no	yes		
Chemical decay	yes	no	no		
Re-suspension	yes	yes	yes		
Inhalation	yes	yes	yes		
Indoor exposure	yes'	no	no		
Onsite exposure	yes	yes	yes⁵		
Short time exposure	yes	no	yes		
Spatial definition	2-D	2-D	2-D		
Surface Water Pathway					
Overland flow (runoff)	yes	yes	yes		
Overland sediment	yes	yes	yes		
Suspended solids	yes	no	no		
Sediment	yes	no	no		
Volatilization	yes	yes	yes		
Spatial definition	2-D	1-D] 1-D		
Ground Water Pathway					
Spatial definition	3-D	3-D	1-D		
Time dependence	yes	yes	yes		
Soil Pathway					
Volatilization	yes	yes	no		
Infiltration	yes	yes	yes		
Ground water loss	yes	yes	l yes		
Degradation	yes	yes	yes		
Soil ingestion	yes	no	yes ³		
Spatial definition	1-D	1-D	no		
Time dependence	yes	yes	ves		

Table 13.1 cont'd. Summary of model features.					
	MEPAS	MMSOILS	PRESTO-EPA-CPG		
Bio-accumulation					
Animals	yes	yes	yes		
Terrestrial plants	yes	yes	yes		
Foliar deposition	ves	ves	ves		
Aquatic organisms	yes	yes	no		
Spatial definition	2-D	2-D	2-D		
Site Data Required	Extensive	Moderate	Moderate		
Contaminant Selection					
Hazardous chemical waste	yes	yes	no		
Radioactive waste	yes	no	yes		
Intakes from Ingestion of					
Drinking Water	yes	yes	yes		
Shower Water	yes	no	no		
Swimming Water	yes	yes	no		
Leafy Vegetables	yes ²³	yes	yes		
Other Produce	yes ²³	yes	yes		
Meat	yes	yes	yes		
Milk	yes	yes	yes		
Finfish	yes	yes	yes		
Shellfish	yes	no	yes		
Special Food	yes	no	eggs		
Shoreline Sediment	yes	no	yes		
Soil	yes⁴	yes	yes		
Intakes from Inhalation					
While Showering	yes	no	no		
Of Air	yes	yes	yes		
Of Re-suspended Soil	yes	yes	yes [*]		
Intakes from Contact					
While Showering	yes	no	no		
While Swimming	yes	no	no		
With Shoreline Sediment	yes	no	no		
With Soil	yes⁴	yes	no		
With Volatiles in Air	yes	no	no		
External Exposures:					
While Swimming	yes	no	no		
While Boating	yes	no	no		
From Air	yes	no	yes		
With Soil	yes	no	yes		
With Shoreline Sediment	yes	no	no		
From Direct Radiation.	yes	no	no		

1. This component not available in 1993 version.

2. From air deposition on crops.

3. From irrigation of crops.

4. Estimations based on either measured concentrations or on calculated accumulations in soil after atmospheric deposition.

5. In the version modified for cleanup scenarios.

6. On-site scenario only.

7. MMSOILS only considers ground surface roughness in wind erosion of particulates.

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