BJC/OR-271

Guidance for Conducting Risk Assessments and Related Risk Activities for the DOE-ORO Environmental Management Program

University of Tennessee

contributed to the preparation of this document and should not be considered an eligible contractor for its review.

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BECHTEL JACOBS COMPANY LLC
managing the
Environmental Management Activities at the
East Tennessee Technology Park
Oak Ridge Y-12 Plant Oak Ridge National Laboratory
Paducah Gaseous Diffusion Plant Portsmouth Gaseous Diffusion Plant
Under contract DE-AC05-98OR22700
for the
U.S. DEPARTMENT OF ENERGY

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ACRONYMS

ARARs	Applicable or Relevant and Appropriate Requirements
BHHRA	Baseline Human Health Risk Assessment
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
COPC	Chemical of Potential Concern
COC	Chemical of Concern
CRE	Center for Risk Excellence
CROET	Community Reuse Organization of East Tennessee
D&D	Decontamination and Decommissioning
DOE	U.S. Department of Energy
EE/CA	Engineering Evaluation/Cost Analysis
ELCR	Excess Lifetime Cancer Risk
EM	Environmental Management
EPA	U.S. Environmental Protection Agency
ES&H	Environmental Safety and Health
ETTP	East Tennessee Technology Park
EUWG	End Use Working Group
FFA	Federal Facilities Agreement
HEAST	Health Effects Assessment Summary Table
HI	Hazard Index
IRIS	Integrated Risk Information System
LMES	Lockheed Martin Energy Systems, Inc.
M&I	Management and Integration
NPL	National Priorities List
OEPA	Ohio Environmental Protection Agency
OREIS	Oak Ridge Environmental Information System
ORNL	Oak Ridge National Laboratory
ORO	Oak Ridge Operations
ORR	Oak Ridge Reservation
PRG	Preliminary Remediation Goal
RAB	Risk Advisory Board
RAGS	Risk Assessment Guidance for Superfund
RAIS	Risk Assessment Information System
RATL	Risk Assessment Technical Lead
RCRA	Resource Conservation and Recovery Act
RFI	RCRA Facility Investigation
RGO	Remedial Goal Option
RI/FS	Remedial Investigation/Feasibility Study
ROD	Record of Decision
TDEC	Tennessee Department of Environment and Conservation
WWW	World Wide Web
Y-12	Oak Ridge Y-12 Plant

EXECUTIVE SUMMARY

The purpose of this document is to establish guidelines to ensure that all risk assessments and related risk activities for the U.S. Department of Energy, Oak Ridge Operations (DOE-ORO), Environmental Management (EM) Program are consistent with both program and regulatory guidance and are technically defensible. This is especially important under the Management and Integration (M&I) contracting process because subcontractors will perform most risk assessment tasks. The use of this document will streamline the completion of human health risk assessments by providing program and project managers with a framework that integrates risk assessment activities into the life cycle of projects.

The methods outlined in this document are consistent with the U.S. Environmental Protection Agency's (EPA) human health evaluation process described in parts A through D of *Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual* (RAGS) (EPA 1989, 1991a, 1991b, 1998). Under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), RAGS serves as the primary regulatory guidance document for all risk assessments and their application to risk management. In addition to RAGS, comments provided by state and federal regulators on previously submitted risk assessment reports and the most up-to-date scientific findings related to the evaluation of human health risk have been incorporated into this document.

This document supercedes *Risk Assessment Strategy at DOE-ORO* (ES/ER/TM-180, LMER 1996c). The material contained herein will be periodically updated as the strategy and risk assessment methodology are revised. The document may be found on-line at the Risk Assessment Information System (RAIS) at http://risk.lsd.ornl.gov/homepage/rap_docs.htm.

1. INTRODUCTION

The U.S. Department of Energy–Oak Ridge Operations (DOE-ORO) is responsible for administering the operations of the Oak Ridge National Laboratory (ORNL), the Y-12 Weapons Plant (Y-12), the East Tennessee Technology Park [collectively referred to as the Oak Ridge Reservation (ORR)], the Portsmouth and Paducah Gaseous Diffusion Plants, and the Weldon Spring Site. As of April 1, 1998, Bechtel Jacobs Company, LLC became the Management and Integration (M&I) contractor for all of the DOE-ORO Environmental Management (EM) Programs with the exception of the Weldon Spring Site. The Weldon Spring Site is administered by the DOE-ORO, and operations there are conducted via a memorandum of understanding with the U.S. Army.

The mission of the DOE's EM Program is:

"...to manage risks to human health and the environment posed by contaminated sites and facilities, legacy waste, and newly generated waste in the most cost-efficient and responsible manner possible to provide for future beneficial reuse." (DOE 1998b)

The primary mission of Bechtel Jacobs Company, LLC is to manage programs in environmental restoration, waste management, technology development and demonstrations, nuclear materials and facilities stabilization and technology transfer for DOE, other federal agencies, and the public. In addition, Bechtel Jacobs Company, LLC is responsible for the reindustrialization of underused buildings, facilities, and land through leases and other mechanisms with the private sector. The successful completion of the Bechtel Jacob's mission involves developing procedures, policies, and guidance to aid program and project managers in making decisions that will ensure the health and safety of workers, the public, and the environment.

Each EM program uses risk assessment to aid in making decisions. Environmental restoration project managers rely on the results of human health and ecological risk assessments, conducted as part of the U. S. Environmental Protection Agency's (EPA) Comprehensive Environmental Response Compensation and Liability Act (CERCLA) Remedial Investigation and Feasibility Study (RI/FS) process, to aid in making decisions regarding the need for and the extent of remediation necessary at a given site. Waste management programs use risk assessment to identify and develop waste acceptance criteria, to determine risks associated with the transport of hazardous materials, and to quantify the long-term risk from wastes disposed at off-site disposal facilities. Technology development and demonstration use risk assessment to evaluate the effectiveness of various treatment technologies for hazardous/radioactive waste. Risk assessment is consistently used throughout the EM program by decision-makers and project managers to ensure the safety and well-being of the employees, the public, and the environment.

In this document, risk assessment is defined as the process that evaluates the potential for adverse health effects resulting from exposure to chemicals (including radionuclides) under a given set of circumstances. Risk assessment is a tool that decision-makers and project managers use to aid in making decisions regarding:

- the treatment, storage, or disposal of hazardous/radioactive materials;
- the need for immediate response to accidental contaminant releases;
- the necessity for clean-up of past and/or on-going contaminant releases;

- the prioritization of projects/activities;
- the establishment of clean-up criteria that are protective of human health and the environment;
- the effectiveness of selected remedies;
- the determination of source terms and estimating probability and magnitude of release due to catastrophic events or deterioration of existing structures or containment systems;
- the effectiveness of treatment technologies; and
- the risk from residual materials, infrastructure, and chemicals in building/structures slated for re-use.

The risk assessment guidelines outlined in the original document, *Risk Assessment Strategy at DOE-ORO* (ES/ER/TM-180, LMES 1996c), have been updated and incorporated into this document. The focus of TM-180 was to ensure that all risk assessment and related risk activities in support of environmental restoration efforts, namely the CERCLA RI/FS process, would be "performed in a consistent and technically defensible manner".

The goal of this document is similar to ES/ER/TM-180, but the scope has been expanded to address other uses of risk assessment and related risk activities that support decision-making [e.g., waste management, decontamination and decommissioning (D&D), technology demonstration, and reindustrialization efforts].

1.1 PURPOSE AND SCOPE

The purpose of this document is to establish guidelines to ensure that all risk assessments and related risk activities for the DOE-ORO EM Program are consistent with both program and regulatory guidance and are technically defensible. This is especially important under the M & I contracting process because subcontractors will perform most risk assessment tasks. The use of this document will streamline the completion of human health risk assessments by providing program and project managers with a framework that integrates risk assessment activities into the life cycle of projects.

The methods outlined in this document are consistent with the U.S. Environmental Protection Agency's (EPA) human health evaluation process described in parts A through D of *Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual* (RAGS) (EPA 1989, 1991a, 1991b, 1998). Under CERCLA, RAGS serves as the primary regulatory guidance document for all risk assessments and its application to risk management. In addition to RAGS, comments provided by state and federal regulators on previously submitted risk assessment reports and the most up-to-date scientific findings related to the evaluation of human health risk have been incorporated into this document.

The Paducah risk assessment guidance document, *Methods for Conducting Human Health Risk Assessments and Risk Evaluations at the Paducah Gaseous Diffusion Plant* (DOE/OR/07-1506&D1, DOE 1996) was prepared to incorporate requirements of the State of Kentucky and EPA Region IV. Although the Paducah risk assessment guidance document references this document, the Paducah guidance is to be considered "site-specific". All risk assessments and risk evaluations at the Paducah Gaseous Diffusion Plant must comply with the requirements outlined in *Methods for Conducting Human Health Risk Assessments and Risk Evaluations at the Paducah Gaseous Diffusion Plant* (DOE/OR/07-1506&D1, DOE 1996) or its most recent revision.

Risk assessments and related risk activities at the Portsmouth Gaseous Diffusion Plant are performed in accordance with the guidelines outlined here, in the Quadrant Resource Conservation and Recovery Act (RCRA) Facility Investigation (RFI) Work Plans, and in the RFI reports that have been approved by the Ohio Environmental Protection Agency (OEPA) and EPA, Region V. Deviations from methods in work plans and reports must be approved by the Risk Advisory Board (RAB), which is defined in Section 1.4, prior to their implementation.

Although risk assessments performed for the DOE-ORO assess the potential threat to human health and the environment from exposure to contaminants, the methods and other information contained herein are specific only to human health risk assessments. The documents entitled *Guide for Performing Screening Ecological Risk Assessment at DOE Facilities* (ES/ER/TM-153, Suter 1995b) and *Approach and Strategy for Performing Ecological Risk Assessments for the Department of Energy Oak Ridge Field Office Environmental Restoration Program* (ES/ER/TM-33R2, Suter 1995a) address the implementation of ecological risk assessments for DOE-ORO.

Additionally, this document does not provide specific guidance for remediation worker risk assessments. Remediation worker safety is of the highest priority to the EM program; therefore, Environmental Safety and Health (ES&H) issues are specifically evaluated and precautions are taken prior to all activities. The ES&H process to safeguard remediation workers is distinctly separate from the estimation of risks to workers under an industrial scenario that is used in decision making and alternative selection. Since remediation workers directly participate in clean-up activities, different parameter values, exposure routes and durations, and toxicity values are chosen to better reflect the workers' circumstances. Workers also face physical safety hazards (e.g., falling, electrocution, etc.) that must be considered. For guidance on conducting a worker risk assessment, refer to *U.S. Department of Energy Worker Health Risk Evaluation Methodology for Assessing Risks Associated with Environmental Restoration and Waste Management* (ORNL-6833, 1995).

1.2 AUDIENCE

This guidance applies to all subcontractors performing risk assessments or related risk activities in support of the DOE-ORO EM M&I Contract. Project Managers and risk assessors are responsible for the consistent application of the guidance as it pertains to risk assessment and related risk activities associated with a specific program or project (e.g., waste management or D&D).

This document will be used to review the risk assessment framework for DOE-ORO EM activities. Program managers, other members of the project team, regulators, and the public may also find this document useful in understanding the important issues in the performance of a risk assessment or other related risk activity.

1.3 IMPLEMENTATION

Risk assessors will be required to follow the guidelines outlined in this document in their statements of work. Deviations from these guidelines will require approval by the project manager and the RAB.

The guidance provided in this document, as well as many of the risk assessment tools identified herein, are available on a publicly accessible World Wide Web (WWW) server as part of the Risk Assessment Information System (RAIS). The RAIS was developed to provide support for the on-going risk assessment and related risk activities of the DOE-ORO both nationwide and internationally. The RAIS is updated and modified as necessary and is maintained under configuration control.

1.4 ROLES AND RESPONSIBILTIES

Project Managers: After projects have been identified (see Section 2) and subcontracts have been awarded, the Bechtel Jacobs Company LLC project managers are responsible for:

- defining the scope of work to be performed,
- ensuring that the statement of work for any subcontracts includes the stipulation that the guidelines outlined in this document are implemented,
- ensuring that the subcontractor identifies a qualified Risk Assessment Technical Lead (RATL) at the onset of the project,
- ensuring that the RATL is qualified to perform/manage the task, and
- approving deviations from the guidelines in this document.

Risk Assessment Technical Lead: The contractor responsible for the risk assessment or related risk activities for a project will appoint a RATL at the onset of a project from within their organization. The RATL is responsible for:

- ensuring that all risk assessment and related risk activities comply with the guidelines outlined in this document,
- ensuring appropriate review by the RAB of any site-specific exposure parameters or scenarios that are developed during the course of a project, and
- ensuring appropriate technical review of risk assessment reports.

Risk Advisory Board: The RAB is comprised of representatives from DOE-ORO; Bechtel Jacobs Company, LLC; and the subcontractors who are currently performing risk assessments or related risk activities for the DOE-ORO. The primary functions of the RAB are:

- to ensure technical review of methodologies, proposed site-specific exposure parameters and scenarios, and risk assessment reports [e.g., RI/FS reports, Engineering Evaluation/Cost Analysis (EE/CAs), and other documents containing an evaluation of risk]; and
- to approve deviations from the guidelines in this document.

1.5 DOCUMENT ORGANIZATION

This document has been organized as follows:

Section 2: The DOE-ORO EM approach to environmental restoration is discussed and differences between the ORR and Paducah and Portsmouth Gaseous Diffusion Plants are noted, including references to guidance materials for Paducah and Portsmouth. Also discussed is the role of risk assessment in the RI/FS process at the ORR.

Section 3: The current environmental management programs are described, and the role of risk assessment in each of these programs is delineated.

Section 4: A more detailed discussion of the risk assessment process is provided,including deviations and clarifications that have been made on Region IV EPA guidance and risk assessment application on the ORR.

Section 5: A detailed discussion of screening risk assessment methods is provided. In particular, screening with risk-based, Preliminary Remediation Goals (PRGs) and integration point assessments are discussed.

Section 6: An overview of baseline risk assessment methods is discussed.

Section 7: An overview of the role of risk assessment in the FS, remedial design/remedial action, Record of Decision (ROD), and five year review of the ROD is outlined.

Section 8: An overview of the tools available on the RAIS World Wide Web site is presented.

The Appendices provide more detailed technical information regarding data evaluation, background comparison, exposure units definition, etc. The appendices are listed below.

Appendix A: Risk Assessment Technical Memoranda
Appendix B: Data Evaluation
Appendix C: Background Comparison
Appendix D: Guide for Air Dispersion Modeling for Risk Assessment
Appendix E: Guide for Groundwater Modeling for Risk Assessment
Appendix F: Food Chain Models for Risk Assessment
Appendix G: Guide for Determining Exposure Units
Appendix H: Uncertainties Associated With the Residential Risk Pathway Models for Soil and Groundwater
Appendix I: Integration Point Assessment Method

2. ENVIRONMENTAL RESTORATION

In *U.S. Department of Energy Environmental Management Program Initial Accelerating Cleanup: Paths to Closure, Oak Ridge Operations Office* (DOE/OR/01-1746, DOE 1998b), the U.S. Department of Energy, Oak Ridge Operations (DOE-ORO) set forth a life cycle cleanup strategy for completing the Environmental Management (EM) Program's mission. Two fundamental principles were adhered to during the development of the cleanup strategy:

1. Accelerating cleanup must not compromise the health and safety of remediation workers or the public or the achievement of appropriate cleanup standards.

2. Efficiencies must occur within the projects and the decision-making process.

Risk assessment will play a key role in ensuring that these two principles are upheld. The clean-up strategy outlines a process that begins with prioritization of subprojects based on their overall risk-benefit value (e.g., risk reduction) and the sequencing of subprojects (in time) to accommodate the budget availability. The life cycle (shown below) continues with the actual implementation of these subprojects followed by an evaluation of risk reduction associated with public health, site personnel safety, and environmental protection.

Risk Ranking → ***Sequencing*** → ***Implementation*** → ***Evaluation***

The risk ranking and sequencing activities are the same for all DOE-ORO facilities; however, the implementation and evaluation of environmental restoration at each facility must address the requirements of all applicable regulatory and interagency agreements (Table 1). Thus, the risk assessment guidelines vary to support environmental restoration efforts.

Table 1. Applicable regulatory and interagency agreements

Facility	Existing Interagency Agreements	Parties	Date
Oak Ridge Reservation	RCRA Hazardous and Solid Waste Amendments Permit	DOE and EPA Region IV	10/22/86
	Federal Facility Agreement for the Oak Ridge Reservation (DOE 1992)	DOE, EPA Region IV, and Tennessee Department of Environment and Conservation (TDEC)	01/01/92
	Toxic Substances Control Act PCB Federal Facility Compliance Agreement	DOE and EPA Region IV	12/16/96
	State of Tennessee Commissioner's Order	DOE and TDEC	10/95
Paducah Gaseous Diffusion Plant	Federal Facility Agreement for the Paducah Gaseous Diffusion Plant (DOE 1998a)	DOE, EPA Region IV, and the Commonwealth of Kentucky	
	Commonwealth of Kentucky Department of Environmental Protection Commissioner's Order	DOE and Commonwealth of Kentucky	10/95
	RCRA Hazardous and Solid Waste Amendments Permit	DOE and Commonwealth of Kentucky (originally issued by EPA Region IV)	08/19/91
	Toxic Substances Control Act Uranium Enrichment Federal Facility Compliance Agreement	DOE and EPA Region IV	02/20/92
	RCRA Toxicity Characteristic Leaching Procedure Federal Facility Compliance Agreement	DOE and EPA Region IV	03/26/92
	CERCLA 106 Administrative Order by Consent	DOE and EPA Region IV	11/88
Portsmouth Gaseous Diffusion Plant	Consent Decree	DOE and the State of Ohio	08/31/89
	Administrative Order by Consent	DOE and EPA Region V	09/27/89, revised 08/04/94
	Toxic Substances Control Act Uranium Enrichment Federal Facility Compliance Agreement	DOE and EPA Region V	10/04/95
	Director of Ohio EPA Final Finding and Order	DOE and the State of Ohio	10/04/95

The following text briefly describes the environmental restoration technical approach for the Oak Ridge Reservation (ORR) and the Portsmouth and Paducah Gaseous Diffusion Plants. This information is provided to illustrate that risk assessment plays a key role in the technical approach for each of the facilities.

Oak Ridge Reservation: Of the five DOE-ORO facilities, three installations [Oak Ridge National Laboratory (ORNL), Y-12 and the East Tennessee Technology Park (ETTP)] comprise the ORR. These installations were constructed in the early to mid-1940s as research, development, and process facilities in support of the Manhattan Project. In addition to the three installations, the ORR also includes the areas within the DOE boundary and buffer zones, land used by the Oak Ridge Associated Universities, and

waterways that may have been contaminated by releases from the DOE-ORO installations. In 1989, the ORR was evaluated by the EPA using the Hazard Ranking System. As a result of this evaluation, the ORR was placed on the National Priorities List (NPL) and was required to comply with the requirements of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) (DOE 1998b).

The ORR strategy for environmental restoration is to accelerate the transition from characterization to remediation by making decisions at the watershed level based on assumed end uses (also referred to as land uses) and existing/historical data. Until recently, the strategy for cleaning up ORR contaminated sites was to investigate each area individually, identify chemicals of concern (and their potential human health and ecological risks) for each site, and assume that the future land use of all sites on the ORR would be unrestricted (e.g., residential, gardening, recreational, etc). The disadvantages of this site-by-site approach are that it is time consuming, not cost-effective, and actions at one site could negatively impact other nearby areas.

The ORR has adopted a new cleanup strategy called "The Watershed Approach". This new strategy involves making cleanup decisions for an entire watershed (a term used to describe a specific area where surface water and often groundwater comprise a specific flow system). Because there are multiple contaminated media and areas within a watershed, this new strategy's cleanup actions rely heavily on the massive amounts of existing/historical and current sampling data. The future land use for a particular watershed (or area within the watershed) will be more accurately and realistically determined by the DOE-ORO, the Tennessee Department of Environment and Conservation (TDEC), the U.S. Environmental Protection Agency (EPA) Region IV, and the public. Cleanup criteria will be based on the recommended future land use.

The watershed cleanup strategy uses a combination of integration point assessments, screening risk assessments, and baseline risk assessments to:

- identify and prioritize contaminated sites and facilities within a watershed,
- determine local area end/land use (relying heavily on existing/historical environmental data), and
- develop an optimum remediation strategy (a remedy) for the identified problems.

Portsmouth Gaseous Diffusion Plant: The Portsmouth Gaseous Diffusion Plant was constructed in the early 1950s to enrich uranium in support of both government and private programs. The plant currently operates under a lease agreement with the U.S. Enrichment Corporation, which produces low-enriched uranium for commercial applications. The DOE is responsible for remedial action to address environmental releases and for decontamination and decommissioning (D&D) of the facilities.

The Portsmouth Gaseous Diffusion Plant is divided into four clean up areas, commonly referred to as quadrants, based on groundwater flow direction. Remediation is accomplished for the quadrants by:

- removing well-defined sources of contamination,

- consolidating and integrating CERCLA-based remedial actions with Resource Conservation and Recovery Act (RCRA) corrective measures and closures for individual or groups of Solid Waste Management Units with common sources or interrelated groundwater plumes,

- using risk-based closure criteria rather than "clean closure criteria" (where practical), and

- establishing cleanup levels and the sequence of cleanup efforts based on risk analysis results.

Paducah Gaseous Diffusion Plant: The Paducah Gaseous Diffusion Plant was constructed in the early 1950's to supply enriched uranium for both government and commercial nuclear fuel needs. Like the Portsmouth plant, the Paducah plant currently operates under a lease agreement with the U.S. Enrichment Corporation, but the DOE is responsible for remedial action to address environmental releases and for D&D of the facilities.

The technical approach for remediation at the Paducah Gaseous Diffusion Plant includes strategies for establishing site priorities, remedial goals based on land use, source control, and remedial actions for groundwater and surface water contamination. Paducah release areas were divided into 30 waste area groups based on common characteristics. These areas were prioritized to focus resources and ensure prompt action in addressing threats to human health and the environment based on the following criteria.

- Mitigate immediate threats in all media, on- or off-site
- Control “hot spots” associated with off-site contamination
- Address suspected sources of off-site contamination
- Address suspected sources of on-site contamination
- Complete final actions for groundwater and surface water integrator units

Summary: Risk assessment is integral to the successful completion of the environmental restoration at each of the facilities, regardless of the differences in the technical approach. Each facility uses risk assessment methods and techniques for:

- risk ranking and sequencing;
- identifying necessary removal, early, and/or final actions;
- establishing clean up criteria and selecting appropriate remedial alternatives; and
- evaluating the effectiveness of selected alternatives.

2.1 PROJECT RISK RANKING

The DOE-ORO EM Program is managed using a comprehensive planning process. In order to assist the EM Program in achieving its mission, the Bechtel Jacobs Company, LLC, Strategy and Regulatory Analysis Group, in conjunction with the watershed project managers, identifies projects based on discrete, definable actions. These projects are then ranked to identify activities that reduce the most significant risks or provide the most value toward achieving the EM mission.

For the DOE-ORO Program, risk ranking determines the relative risk of each project in terms of public safety and health, environmental protection, and site personnel safety and health. Risk ranking is conducted quantitatively, incorporating available baseline and screening risk assessments using the Environmental Management Benefit Assessment Matrix. The matrix provides a consistent, systematic framework for evaluating and quantifying the before score, after score, and net benefit for each project. From the net benefit score, the projects can them be ranked on the basis of relative risk. Technical data and risk rankings for each activity are maintained in the Environmental Management Risk Ranking database. More detailed information on the Environmental Management Benefit Assessment Matrix and the risk ranking process can be found in *Department of Energy - Oak Ridge Operations Environmental Management Program Risk Ranking Methodology* (DOE 1998c).

Risk ranking assists DOE management in sequencing projects over time. The sequencing process considers the risk ranking score, regulatory milestones, logical progression of cleanup, mortgage reduction (i.e., reduction of life cycle costs), mission impacts, and stakeholder concerns in order to establish program budget priorities. The results of the sequencing support the development of EM budget

requests. Included with the annual budget request is an Integrated Priority List, which ranks projects in order of priority. The Integrated Priority List is determined by reviewing the baseline sequence for the fiscal year, current budget information, and additional concerns specific to the fiscal year.

Note: As previously stated, both the Paducah and Portsmouth Gaseous Diffusion Plants have documented site-specific risk assessment guidance related to the implementation of the CERCLA and/or RCRA processes. Therefore, the remainder of this section addresses the implementation of risk assessment and related risk activities on the Oak Ridge Reservation only.

2.2 IMPLEMENTING THE RI/FS PROCESS

DOE is responsible for cleaning up the ORR by following the CERCLA RI/FS process. Section III.A.1 of the Federal Facility Agreement (FFA) requires DOE to assess the impacts of Oak Ridge Reservation areas on human health and the environment (DOE 1992). To fulfill this requirement, sites must be identified and evaluated to determine whether response activities are needed. DOE has established a specific RI/FS approach aimed at categorizing sites (Fig. 1) so that the CERCLA process is accelerated and areas where no further investigation is required are de-listed from the NPL. The approach involves:

- conducting screening area evaluations by reviewing available information and performing area reconnaissance to identify potential release areas and/or areas of contamination,
- conducting removal site evaluations to determine whether a removal action is appropriate immediately,
- conducting remedial site evaluations to determine whether further study is needed for identification of appropriate response actions, and/or
- conducting studies (e.g., RI/FS) to support decision documents for response actions.

Each of these activities involve either a qualitative or quantitative evaluation of the risks posed to human health and the environment from exposure to chemicals/conditions at each site. Section 4 of this document presents a discussion of the risk analysis methods to be used during each of these evaluations. The categories of sites are listed in Table 2.

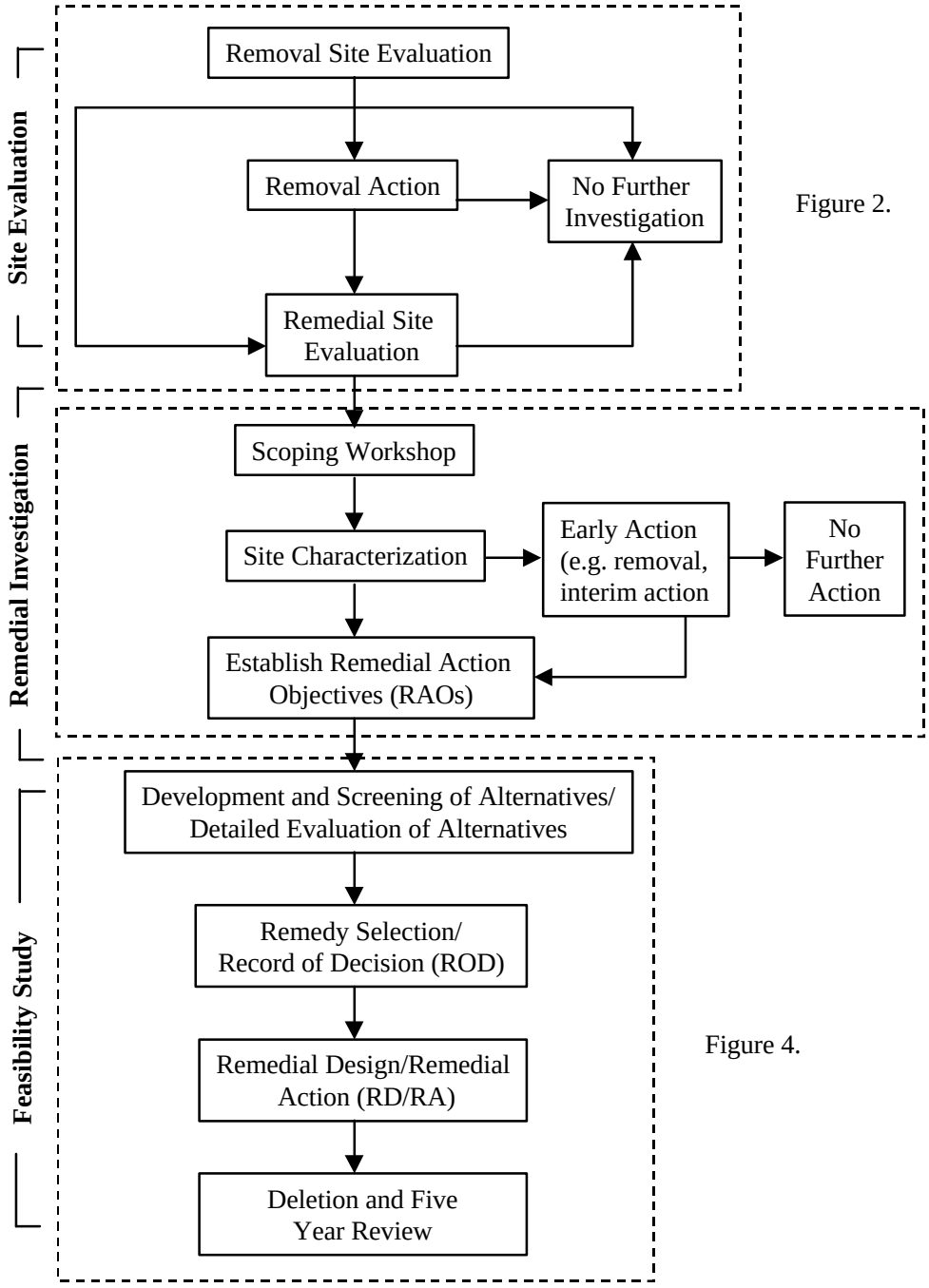


Figure 2.

Figure 3.

Figure 4.

Figure 1. DOE-ORO Remedial Investigation/Feasibilty Study process

Table 2. Site categories

Categories	Criteria for sites in each category
Operable Units	CERCLA actions that have been defined in approved decision documents (e.g., record of decision, Action Memorandum).
Characterization Areas	Sufficient information exists to recognize that additional CERCLA action is appropriate.
Remedial Site Evaluation Areas	Some existing/historical information exists to conclude that the area has a high potential of being contaminated; however, insufficient information exists to determine if further investigation or remediation is warranted.
Removal Site Evaluation Areas	The site meets criteria for evaluation to be considered under CERCLA (i.e., area is inactive and hazardous substances have been released or a threat of a release exists), but insufficient information exists to determine if a removal or remedial action is necessary.

2.2.1 Site Evaluations

Two types of site evaluations are conducted on the ORR: removal site evaluations and remedial site evaluations (Fig. 2). Removal Site Evaluations are conducted for those sites that are considered "newly discovered", meaning that they were not previously listed as source areas in Appendix C of the *Federal Facility Agreement for the Oak Ridge Reservation* (DOE 1992). The removal site evaluation may involve a limited environmental sampling, but typically it is performed using available analytical data. The available data are compared with risk-based Preliminary Remediation Goals (PRGs) and may indicate that:

- a removal action is warranted,
- a remedial site evaluation should be performed, or
- no further investigation is needed.

Note: Sometimes, emergency and time-critical removal actions are not formally established as projects until after actions are taken, because of the immediate need to protect human health and the environment. Sites identified as requiring a non-time critical removal or remedial action, however, are established as projects and must then undergo prioritization.

Remedial Site Evaluations are conducted if the available existing/historical data and operational information indicate that there is the potential for environmental contamination, but insufficient or poor quality data require the determination of whether additional investigation (e.g., data collection) or remediation is warranted. In such cases, a comparison of data to risk-based PRGs is a tool project managers can use to:

- identify data needs and limitations (e.g., detection limits are greater than risk-based PRGs),
- focus future sampling and analysis on chemicals and exposure pathways of potential concern,
- establish appropriate detection limits for subsequent environmental sample analysis,
- support a No Further Investigation Determination, and/or
- quantitatively support the need for additional study.

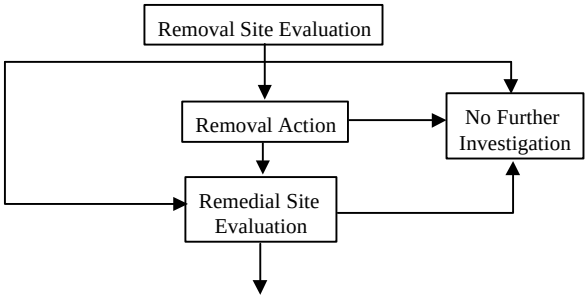


Figure 3

Site Evaluation and Risk Assessment

Screen data against risk-based preliminaryremediation goals to:

- prioritize activities,
- identify data gaps and limitations,
- focus future sampling and analysis on contaminants and pathways of concern,
- establish appropriate detection limits for subsequent environmental sample analysis,
- provide risk information on which to base removal action, if necessary,
- provide risk information on which to base risk reduction resulting from removal,
- support a no further investigation determination, and
- quantitatively support the need for additional study.

Figure 2. The site evaluation process and risk assessment

2.2.2 Remedial Investigation

The Remedial Investigation phase of the ORR's RI/FS process begins with a scoping workshop (sometimes referred to as a data quality objectives workshop) (Fig. 3). The scoping workshop is attended by the DOE EM Managing and Integrating (M&I) contractor project team, the DOE Program Manager, TDEC, and EPA Region IV team members. The purposes of this workshop are to:

- develop conceptual site models (for the movement of chemicals in the geology and hydrology and for the human health and ecological risk assessments);
- identify preliminary remedial action objectives and likely response actions;
- identify Applicable or Relevant and Appropriate Requirements (ARARs) and risk-based PRGs;
- determine the type of decisions to be made, and the type, quantity, and quality of data needed to support those decisions (i.e., define Data Quality Objectives);
- identify the need and schedule for treatability studies (as necessary);
- design the data collection program (e.g., sampling approach, analytical methods, and detection limit requirements); and
- define the RI and FS tasks (i.e., the scope of work to be performed).

Based on the results of the scoping workshop, a RI work plan is developed and submitted for approval. Once approved, the workplan is implemented. The results of the site characterization activities are documented in the RI Report, which includes the baseline human health risk assessment. The conclusions of the baseline human health risk assessment are used to:

- help determine whether additional response actions are necessary,
- provide evaluations of the effectiveness of prior actions (i.e., comparison of current and historical data) (if appropriate),

- document the magnitude of risk and the primary causes of that risk, and
- define Remedial Goal Options (RGOs).

Note: During the preparation of the baseline human health risk assessment, newly acquired data will be incorporated in the watershed database and the modified data set will again be compared to risk-based PRGs. This comparison may result in the identification of early actions (including removals and interim actions) in order to reduce risks and/or accelerate the clean-up process.

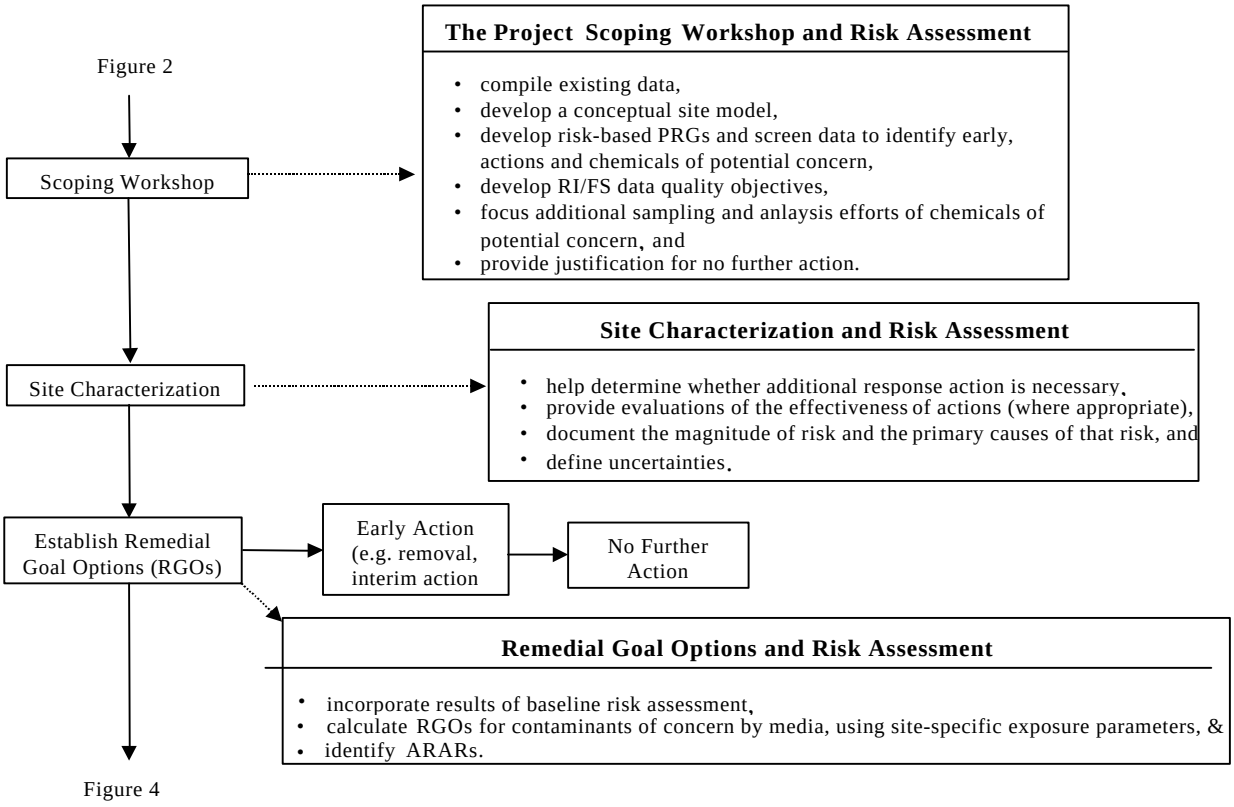


Figure 3. Site characterization and risk assessment

2.2.3 Feasibility Study

The selection of an appropriate remedial action begins with a screening of potential alternatives during the initial scoping workshop. This is conducted prior to the development of the RI work plan (Fig. 4). The preliminary screening of alternatives is refined as more information becomes available and the results of the baseline ecological and human health risk assessments determine the chemicals and pathways of concern. During the selection of remedial actions, short-term and long-term risks must be considered. The analysis of short-term risks focuses on the potential adverse effects on human health and the environment from implementation of the remedial action. The analysis of long-term risks focuses on the risk that will remain after remedial action has been taken (this level of remaining risk is termed residual risk). These analyses may be either qualitative or quantitative, depending on site conditions. For more information, refer to page 14 of *Risk Assessment Guidance for Superfund, Part C* (EPA 1991b).

The results of these risk analyses are presented in the FS Report. Table 3 illustrates the differences between the baseline human health risk assessment and the risk evaluation of alternatives.

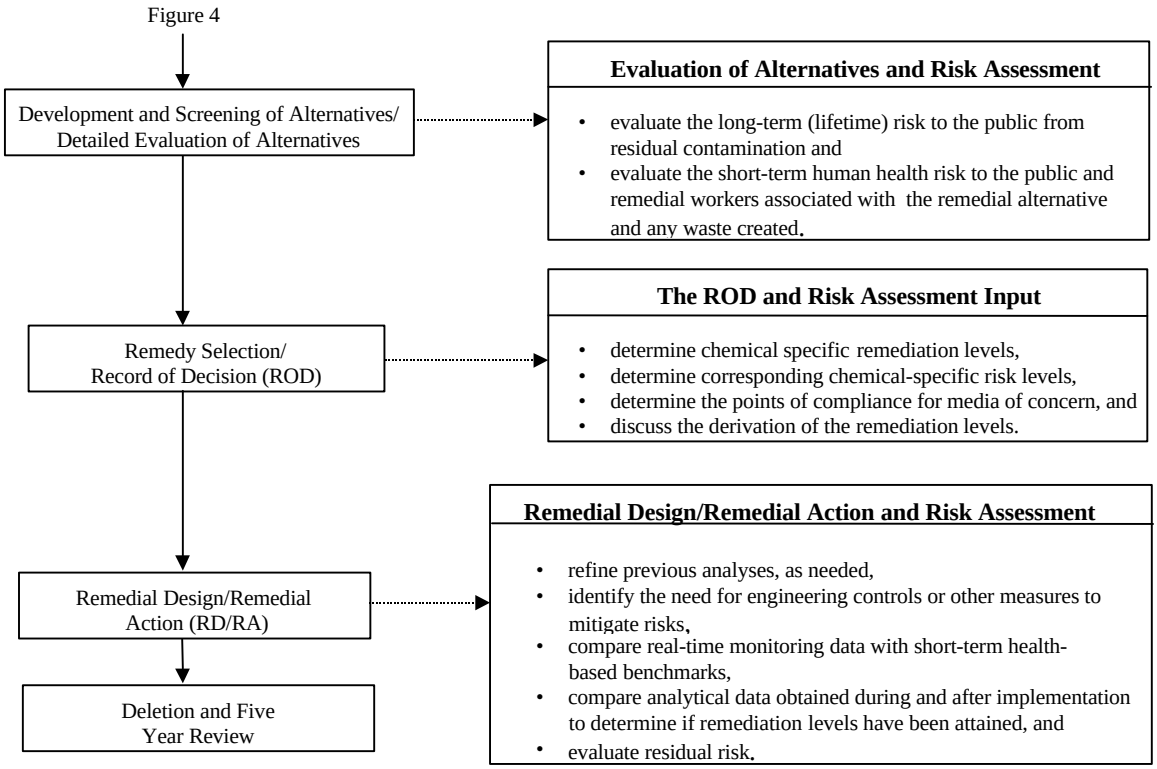


Figure 4. The feasibility study and risk assessment

Table 3. Comparison of the baseline human health risk assessment and the risk evaluation of alternatives

	Baseline Human Health Risk Assessment (quantitiative)	Risk Evaluation of Alternatives (may be quantitative or qualitiative)
Contaminant Sources	Uncontrolled site	Remedial activity and residual contamination May include chemicals not present under baseline conditions (e.g., those created during remediation)
Timing of Releases	Releases due to natural processes (e.g., leaching, weathering)	Releases due to implementation of remedy
Exposed Populations	Current and potential future	Current, remediation workers, and potential future (if residual risks are present)
Duration	Includes lifetime exposure	Long-term includes lifetime exposure Short-term only includes less-than-lifetime exposure

Assessment of Short-term and Long-term Risks for Remedy Selection DOE/EH-413/9708 (DOE 1997)

2.2.4 Deletion and Five Year Review

A five-year review of the record of decision for a site (or areas and media within the watershed) is conducted if the selected remedial action(s) results in residual hazardous substances, pollutants, radionuclides, or chemicals. The purpose of this review is to ensure that the long-term effectiveness of

the remedy continues to protect human health and the environment. The rigor of these assessments is dependent on the amount of additional analytical information and ranges from a simple review of existing information to development of a new risk assessment (if site conditions warrant). These reviews will continue to occur as long as residual contamination is present or until the DOE, TDEC, and EPA Region IV decide otherwise.

3. OTHER ENVIRONMENTAL MANAGEMENT ACTIVITIES

There are other programs in addition to environmental restoration that fall under the purview of the U.S. Department of Energy, Oak Ridge Operations (DOE-ORO) Environmental Management (EM) Program: waste management, decontamination and decommissioning (D&D), technology development and demonstration, and reindustrialization. Each of these programs uses risk assessment methods and techniques to support decision-making. The following text briefly describes the risk-related activities that are performed for these programs and illustrates the need for active involvement.

3.1 WASTE MANAGEMENT

Waste management activities include categorizing wastes (e.g., sanitary, hazardous, low-level radioactive, mixed waste, etc.) to meet disposal criteria under the Resource Conservation and Recovery Act (RCRA), the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), DOE Orders, or other regulatory drivers; evaluating the feasibility of on-site versus off-site disposal (including an evaluation of transportation risk); waste reduction efforts; and overall protection of waste management/remedial workers and the public.

Risk assessment methods in waste management are used to:

- derive estimates of waste volumes and the associated risks/hazards,
- evaluate transportation risk,
- estimate risk from process waste streams and evaluate the cost/benefit of various waste reduction efforts,
- perform cost/benefit analyses of remedial alternatives,
- evaluate worker risk and risk to the public from disposal activities, and
- develop a Waste Acceptance Criteria Screening process that complies with DOE Orders and the risk goals established under CERCLA and RCRA for the reclassification of radioactive waste so that it may be release to a Subtitle C or D landfill.

3.2 DECONTAMINATION & DECOMMISSIONING

The DOE and the U.S. Environmental Protection Agency (EPA) issued a joint policy [*Policy on Decommissioning Department of Energy Facilities Under CERCLA* (DOE and EPA 1995)] that addresses the implementation of CERCLA at D&D facilities. The policy established that decommissioning activities will be conducted as non-time-critical removal actions where appropriate. This approach recognizes that demolition activities are typically straight forward with limited alternatives available for consideration. The evaluation process conducted prior to the implementation of a non-time-critical removal, as well as the engineering alternatives, are documented in the Engineering Evaluation/Cost Analysis report. Per guidance from the EPA (EPA 1993) and DOE (DOE 1994, 1997), a streamlined risk evaluation is conducted to focus the remedial action on the specific problem or the existing/imminent health or environmental threats rather than address all potential exposure pathways; therefore, the streamlined risk evaluation may be limited in scope compared to a conventional baseline risk assessment.

Streamlined risk evaluations can be used to justify a removal action and to identify current or potential exposures that should be prevented. It is important to remember that the level of complexity of a streamlined risk evaluation is based on the action to be undertaken and may in some cases require as much effort as a conventional baseline risk assessment.

Risk guidance for D&D facilities was developed by DOE-ORO with the assumption that the facilities may need to be evaluated with the same rigor as DOE-ORO hazardous waste sites. Therefore, the guidance provides methods to estimate:

- the potential source terms associated with past and/or on-going releases from available historic, operational, and environmental data;
- the probability and magnitude of releases due to catastrophic events (e.g., tornadoes); and
- the potential magnitude of releases due to deterioration of building materials with time.

These estimates can be used, in turn, to complete screening risk evaluations, baseline risk assessments, and alternatives evaluations.

The screening risk evaluation guidance was designed to produce relative risk scores to support D&D action, prioritization, and decision-making. The baseline risk assessment guidance was developed using parts A through C of *Risk Assessment Guidance for Superfund* (EPA 1989, 1991a, 1991b) to provide a consistent approach for projecting the potential for adverse effects to human health and the environment from D&D facilities. These unique documents provide methods to estimate source terms from historical and operational information regarding the nature and volume of materials contained within the infrastructure (e.g., piping, insulation, drains, etc.). The D&D risk assessment guidance documents are referenced in Table 4, and a brief abstract for each is provided in Appendix A.

Table 4. D&D risk assessment guidance documents

Baseline Risk Assessment Guidance for D&D Facilities, K/ER-153/R1, Oak Ridge National Laboratory, Oak Ridge, Tennessee. (LMES 1995a)
D&D Alternatives Risk Assessment Guidance, Oak Ridge National Laboratory, Oak Ridge, Tennessee. DRAFT (LMES 1996a)
D&D Screening Risk Evaluation Guidance, ES/ER/TM-165, Oak Ridge National Laboratory, Oak Ridge, Tennessee. (LMES 1995b)

The methods outlined in the D&D guidance documents may be used to support a streamlined risk evaluation. The D&D guidance documents provide information for data evaluation, source term estimation, exposure assessment, catastrophic failure, and other related risk activities (i.e., prioritization, evaluation of alternatives, etc.). This information helps ensure that risk assessments are consistent with accepted regulatory guidelines and technically defensible. The guidance is not all encompassing, however, as new risk assessment methods are being developed in the D&D area. The Risk Assessment Technical Lead (RATL) for a particular project should consult with the project manager and the Risk Advisory Board (RAB) as needed to ensure that:

- the most innovative and cost effective methods of assessment are used for D&D risk evaluations,
- the new methods are consistent with existing regulatory guidance, and
- the assessment will meet the needs and expectations of the DOE-ORO EM Program.

3.3 TECHNOLOGY DEVELOPMENT AND DEMONSTRATION

Prior to the passage of CERCLA, remedial technologies were limited to those effective at addressing current problems and to land disposal of waste. The requirements of CERCLA necessitated the development of innovative technologies that provide long-term effectiveness and permanence. The goal of DOE-ORO's technology development and demonstration programs are to develop treatment technologies that meet regulatory requirements, can be demonstrated at DOE facilities, and can be ultimately transferred to use in the private sector.

Risk assessment input to the evaluation of treatment technologies occurs primarily in the evaluation of effectiveness. The technology must reduce the toxicity, mobility, or volume of the waste in order to be considered effective. In addition, a comparison between alternatives may be conducted to determine their relative costs/benefits.

3.4 REINDUSTRIALIZATION

In January 1996, DOE began the process of reindustrialization at the East Tennessee Technology Park (ETTP). Several leases have been signed with the Community Reuse Organization of East Tennessee (CROET), which in turn subleases both land and facilities to private sector firms or other organizations. The current uses of these properties include commercial, industrial, or business.

Prior to leasing a property, the CROET and DOE-ORO sign a Memorandum of Understanding, which states that all parties agree to the objective of leasing a specific piece of property (land or facility) for a defined use. After the Memorandum of Understanding is signed, DOE reindustrialization staff prepare a Baseline Environmental Analysis Report that is modeled after the requirements in CERCLA Section 120 (h). This report establishes a baseline condition of the facility and identifies hazardous materials (per 40 Code of Federal Register 373) that are present, stored, or have been released at the facility or land area. This baseline report is accompanied by a screening-level human health risk assessment when appropriate. DOE-ORO submits these reports to TDEC and EPA Region IV. The screening risk assessments use existing/historical data for a facility and/or land area to:

- provide an analysis of risks/hazards in order to support the determination that the facility/land area is safe for occupation by a tenant; and

- screen high risk/hazard areas from the lease or identify high risk/hazard areas within the lease space on which to impose constraints and access restrictions.

The potential contamination surrounding the lease space (either outside a facility or in an area adjacent to the lease area) is also assessed to determine potential impacts on tenants. Similar to the risk approach for D&D facilities, the screening risk assessments for reindustrialization are based on the CERCLA risk methodology (Section 4). These screening risk assessments incorporate the available D&D guidance, as necessary, to meet the needs of the particular leased space. For example, methods described in the *Baseline Risk Assessment Guidance for D&D Facilities* (LMES 1995a) may be used to develop the source term for a particular facility under consideration for lease.

4. RISKASSESSMENT IMPLEMENTATION

Risk assessments and risk-related activities undertaken in support of the U.S. Department of Energy, Oak Ridge Operations (DOE-ORO) follow the regulatory guidance documents listed in Table 5, the technical memoranda listed in Appendix A, and "site-specific" guidance. Generally, the "site-specific" guidance presented in the following subsections has been developed to:

- address the use of existing/historical data;
- incorporate land use determinations;
- define the use of screening and integration point assessments;
- select scenarios, pathways, chemicals, and media of concern; and
- identify risk assessment tools available for use by all subcontract personnel.

A risk assessment consists of four distinct steps: data collection and evaluation, exposure assessment, toxicity assessment, and risk characterization. The outcome of a risk assessment is either a set of chemicals, pathways, media, and/or scenarios of concern for which an appropriate action must be undertaken or a determination that no action is required. The following sections briefly describe the steps of a risk assessment and define the "site-specific" guidance related to each step.

Table 5. Risk assessment regulatory guidance documents

Appendix D of *Risk Assessment Guidance for Superfund, Vol. 1,* ("Corrections to RAGS—Part B, Sections 3.3.1 and 3.3.2"). (EPA 1991d)
Dermal Exposure Assessment: Principles and Application, Interim Report. EPA/600/8-91/011B, Office of Research and Development, Washington, D.C. (EPA 1992)
Exposure Factors Handbook, Volume I, II, and III, EPA/600/P-95/002Fa, Office of Research and Development, National Center for Environmental Assessment, Washington, D.C. (EPA 1997)
Guidance for Data Usability in Risk Assessment, EPA/540/G-90/008, Office of Emergency and Remedial Response, Washington, D.C. (EPA 1990)
Risk Assessment Guidance for Superfund: Volume 1, Human Health Evaluation Manual (Part A), EPA/540/1-89/002, Office of Emergency and Remedial Response, Washington, D.C. (EPA 1989)
Risk Assessment Guidance for Superfund: Volume 1, Human Health Evaluation Manual (Part B, Development of Risk-based Preliminary Remediation Goals), OSWER Directive 9285.7-01B, Office of Emergency and Remedial Response, Washington, D.C. (EPA 1991a)
Risk Assessment Guidance for Superfund: Volume 1, Human Health Evaluation Manual (Part C, Risk Evaluation of Remedial Alternatives), OSWER Directive 9285.7-01C, Office of Emergency and Remedial Response, Washington, D.C. (EPA 1991b)
Risk Assessment Guidance for Superfund: Volume 1, Human Health Evaluation Manual (Part D, Standardized Planning, Reporting, and Review of Superfund Risk Assessments), OSWER Directive 9285.7-01D, Office of Emergency and Remedial Response, Washington, D.C. (EPA 1998)
Standard Default Factors, OSWER Directive 9285.6-03, Office of Emergency and Remedial Response, Washington, D.C. (EPA 1991c)
Supplemental Guidance to RAGS: Region 4 Bulletins, Human Health Risk Assessment, Waste Management Division, Office of Technical Services. (EPA 1996)

4.1 DATA EVALUATION

The first step in the risk assessment process, regardless of the type of risk assessment to be performed (i.e., screening, integration point assessment, baseline), is data collection and evaluation. The quantity and quality of available environmental data often determine the level of evaluation (i.e., remedial site evaluation versus remedial investigation, or screening assessment versus baseline assessment) to be performed. The current DOE-ORO technical approach to remedial action is to rely heavily on existing/historical data in order to reduce cost and accelerate clean-up, disposal, or reuse. This strategy may be further streamlined by employing a phased approach to data collection; additional data is collected in phases until an appropriate technical decision can be made.

Prior to implementation of any risk assessment or related risk activity, all relevant existing/historical data are obtained from the project environmental data coordinator or the Oak Ridge Environmental Information System (OREIS). This system is a centralized, standardized, quality-assured, and configuration-controlled environmental data management system. The primary mission of OREIS is the efficient retrievability and long-term retention of consolidated DOE-ORO environmental data generated by the environmental restoration, compliance, and surveillance activities at the Oak Ridge Reservation (ORR). To achieve this mission, OREIS:

- contains both existing/historical data and data from ongoing activities;
- maintains data in a standardized, quality assured, and configuration controlled information system;
- includes known quality measurement and spatial data from environmental media (e.g., groundwater, surface water, sediment, soil, air, and biota) as well as descriptive and qualifier metadata;
- maintains data for the five DOE-ORO facilities; and
- fulfills DOE-ORO's environmental information management obligations under an enforceable Federal Facility Agreement (FFA) Docket No. 8904FF under Section 120 of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) and Sections 3008(h) and 6001 of the Resource Conservation and Recovery Act (RCRA).

Obtained data are subjected to a data usability evaluation (Appendix B). This evaluation generally follows the guidelines outlined in both *Risk Assessment Guidance for Superfund, Part A* (RAGS) (EPA 1989) and *Guidance for Data Usability in Risk Assessment* (EPA/540/G-90/008) (EPA 1990). The purpose of this evaluation is to:

- determine if the existing/historical data meet the requirements of the project data quality objectives,
- identify any data needs that may exist (e.g., lack of data for certain environmental media or time periods),
- develop a list of chemicals of potential concern,
- focus additional sampling efforts (if any) on chemicals of potential concern,
- ensure that method detection limits are sensitive enough to detect concentrations less than risk-based Preliminary Remediation Goals (PRGs), and

- ensure that data collection activities support the project data quality objectives.

The site-specific data set is evaluated to ensure that the quality of the data is appropriate based on the project-specific data quality objectives. If the data evaluation has not been completed in earlier phases of the investigation, it may be completed as part of the risk assessment. Appendix B contains detailed guidance for conducting the data evaluation and determining the chemicals of potential concern (COPCs) for quantitative risk assessments. In general, the data evaluation performed for risk assessment purposes consists of the following steps.

- **Evaluate analytical methods, quantitation limits, qualifiers and codes, and blanks.** The risk assessor performs the following actions, regardless of whether the data have or have not been validated by an independent party or if the action items have already been performed.

  — Evaluate the data set to ensure that the analytical methods were appropriate for the chemical analyzed and the sample matrix.

  — Evaluate the quantitation limits to ensure that the detection limits were not unusually high.

  — Evaluate the qualifiers and codes to ensure that the data are valid.

  — Evaluate and perform a comparison of blank concentrations to actual sample concentrations to ensure that the concentrations were not biased by either the laboratory preparation methods or the analytical methods.

- **Determine if tentatively identified compounds are significant.** Tentatively identified compounds are retained as chemicals of potential concern only if they are detected frequently and have been associated with site operations.

- **Compare data set to background and reference samples.** A comparison of sample concentrations with available background concentrations is useful for identifying non-site-related chemicals and radionuclides. The background values represent naturally-occurring levels of chemicals that are present under ambient conditions (i.e., not influenced by anthropogenic sources). In general, this comparison is applicable only to inorganic chemicals and a select number of radionuclides. Information specific to the ORR background concentrations is listed below.

  — Soil background concentrations for the ORR were obtained from a comprehensive effort. The soils data obtained from this effort are presented in the *Final Report on the Background Soil Characterization Project at the Oak Ridge Reservation, Oak Ridge, Tennessee, Volumes 1–3* (DOE 1993). These data are used to screen environmental data sets and eliminate contaminants determined to not exceed background concentrations.

  — Chemicals eliminated as a result of background or reference sample comparisons are discussed in the text of the baseline risk assessment report. Appendix C presents detailed guidelines on statistical approaches that can be used to compare site-specific data and background.

  — Groundwater background concentrations do not exist for all of the ORR; however, background concentrations for inorganic chemicals in groundwater at the Y-12 Plant were developed using groundwater data collected under the Y-12 Groundwater Monitoring Program. The methodology used to develop these background concentrations and the values themselves are contained in *Determination of Reference Concentrations for the inorganic Analytes in Groundwater at the U.*

S. Department of Energy Oak Ridge Y-12 Plant, Oak Ridge, Tennessee, (Y/ER-234, LMES 1996b).

Note: Due to the diverse subsurface environment of the Oak Ridge Reservation, there are many uncertainties associated with background concentrations. Therefore, background data sets should only be used after all parties agree to their validity and pertinence to the investigated problem.

- **Eliminate essential nutrients.** Those contaminants that are considered to be essential nutrients are eliminated from the quantitative evaluation if they are not considered to be significantly elevated and/or if no toxicity information is available. The only chemicals which may be eliminated as essential nutrients are calcium, chloride, iodine, magnesium, phosphorus, potassium, and sodium (EPA 1996).

- **Perform risk screening using chemical-specific, risk-based PRGs.** For each exposure pathway, analytes are compared to chemical-specific PRGs for the residential scenario. The pathways included in the derivation of these PRGs are those deemed necessary to support remedial decisions. Analytes for which the maximum detected concentrations are less than chemical-specific PRGs at concentrations posing *de minimis* risk (i.e., risk ≤ 1E-06 or Hazard quotient ≤ 0.1 or if risk ≤ 1E-06 *and* Hazard quotient ≤ 0.1) for the residential scenario may be eliminated from the quantitative risk assessment. In addition, if no chemical, land use scenario, or pathway exceeds the most conservative PRG, any or all of the site, land uses scenarios, or pathways may be designated no action (i.e., PRG screen is sufficient to support no action). The Risk Assessment Information System (RAIS) provides a means to calculate risk-based PRGs using standard exposure equations for a number of exposure pathways. This interactive web program allows the user to select the chemicals for which PRGs are needed and to customize the exposure equations for the routes to be evaluated. For more information, visit the web page at: http://www.risk.lsd.ornl.gov/prg/prg_search.html.

- **Compare nondetected chemical quantitation limits to PRGs.** The reported detection limits for all nondetected chemicals (i.e., analytes that are not detected in any/all samples) are compared to PRGs to ensure that the detection limits are appropriate. A table is generated as a result of this comparison, and the results are discussed in the text of the report.

- **Compile the list of COPCs.** All chemicals that remain after the previous steps have been performed are compiled in a list of COPCs. This list of chemicals is carried through the risk assessment and is the basis for any remedial decisions.

4.2 EXPOSURE ASSESSMENT

An exposure assessment is the determination or estimation (qualitative or quantitative) of the magnitude, frequency, duration, and route of exposure for each potential or actual receptor population to be evaluated in the risk assessment. During the exposure assessment, the risk assessor:

- characterizes the exposure setting to identify the potentially exposed receptors, their activity patterns, and any other characteristics that might increase/decrease their likelihood of exposure;

- identifies exposure routes (develops a conceptual site model) and scenarios;

- estimates the exposure concentration; and

- calculates a chemical-specific intake or dose.

Once the appropriate exposure routes and scenarios have been identified, the risk assessor must select the appropriate dose equations and associated parameter values. The dose equations are used to calculate either the amount of contaminant that is in contact with the body at an exchange boundary per unit body weight per unit time or the amount of contaminant that is absorbed by the body per unit body weight per unit time. The output of this activity is used in conjunction with the output from the toxicity assessment to quantify potential risks/hazards to receptors during the risk characterization. Equations and their associated parameter values for many of the exposure pathways pertinent to the evaluation of risk/hazard on the ORR and at Portsmouth and Paducah are available on the RAIS at the web address provided in Section 4.1.

The following subsections outline exposure assessment guidance that has been developed for sites on the ORR. Much of this guidance is specific to the remedial investigation/feasibility study process, but it is also of use for other risk assessment activities on the ORR (e.g., the discussion concerning land use).

4.2.1 Characterization of the Exposure Setting: Land Use

The end use (land use) of any site, whether it is a burial ground, a pond, or building, is critical to the evaluation of risks/hazards associated with that area. The future use of an area determines the exposure pathways and associated equations and parameter values, regardless of the level of the assessment (e.g., screening, integration point, or baseline). The DOE-ORO, the Tennessee Department of Environment and Conservation (TDEC), and the U.S. Environmental Protection Agency (EPA) recognize that land use determination on the ORR must incorporate the community values and their desired future uses for the ORR. Therefore, in 1996, DOE asked the ORR Environmental Management Site Specific Advisory Board to form a committee to solicit input from the community and make recommendations on the future use of the ORR. This committee is called the End Use Working Group (EUWG).

In July, 1998, the EUWG published *Final Report of the Oak Ridge Reservation End Use Working Group* (EUWG 1998). Overall, the EUWG developed four types of recommendations:

- community guidelines for contaminated land and water on the ORR,
- end uses for the five ORR watersheds and several areas not currently included in the watersheds,
- construction of an on-site ORR disposal facility, and
- long-term stewardship of contaminated land.

The land use categories and the criteria used by the EUWG in making recommendations are presented in Table 6. Likewise, the land use categories used by the DOE for planning and evaluation purposes in the *Initial Accelerating Cleanup Paths to Closure Oak Ridge Operations Office* (DOE 1998b) are presented in Table 7. Although similar, the EUWG and DOE categories and their respective definitions vary enough that a decision regarding their influence on the selection of future exposure routes and scenarios must be made prior to the development of the human health conceptual site model. Recommendations for specific sites (including remedial action, D&D, and areas slated for reuse) are included in each of the documents.

Table 6. End Use Working Group End Use Criteria

End Use Category	Surface Use	Depth of Clean Soil	Groundwater Use	Surface Water Use	Ownership
Unrestricted	Unrestricted	Unlimited	Unrestricted	Unrestricted	Government or Private
Uncontrolled Industrial	Industrial	10 feet	Not Allowed	Unrestricted	Government or Private
Recreational	Recreational	2 feet	Not Allowed	Recreational Uses	Government or Private
Controlled Industrial	Industrial with restrictions	2 feet, additional evacuation by permit	Not Allowed	Not Allowed	Government or Private
Restricted Waste Disposal	Limited to monitoring and maintenance	No soil disturbance allowed	Not Allowed	Not Allowed	Government

Table 7. *Paths to Closure* End Use Scenarios

Category	Definition
Unrestricted	Unfenced areas where subsistence or commercial agriculture predominates without restriction on surface water or groundwater use or where permanent residential use predominates without restriction on surface water with the possibility of groundwater restrictions.
Restricted Industrial	Active industrial facility where groundwater use may be restricted.
Open Space/Recreational	Posted areas are generally reserved as buffer or wildlife management zones. Native Americans or other authorized parties may be allowed permits for occasional surface area use. Access to or use of certain areas may be prevented by passive barriers (e.g., where soil is capped). Limited hunting or livestock grazing may be allowed. Unfenced areas permit daytime use for recreational activities (e.g., hiking, biking, sports), hunting, and some overnight camping. Fishing may be limited to catch-and-release.
Controlled Access	DOE maintains restricted access areas for secure storage and disposal of nuclear materials or waste. Barriers and security fences prevent access by unauthorized persons. Wildlife and plants are controlled or removed.

4.2.2 Identification of Exposure Pathways

For exposure to occur, a source of contamination or contaminated media must exist that serves as a point of exposure or that transports chemicals away from the source to a point where exposure could occur. In addition, a receptor must come into direct contact (i.e., ingestion, inhalation, dermal contact, external exposure) or indirect contact (such as ingestion of foodstuffs that have bioaccumulated chemicals within their systems) with the contaminant. This concept is referred to as an exposure pathway. The elements of an exposure pathway are source, environmental transport/transfer media, exposure point, exposure route, and receptor. Once a decision has been reached on land use for a site, the exposure pathways can be identified.

Based on the activity patterns of a population, there may be more than one exposure pathway for any given individual. Therefore, the exposure assessment must include an evaluation of the activity patterns of the potential receptors to determine what combination, if any, of exposure pathways could affect an

individual. This evaluation results in the generation of exposure scenarios. Exposure scenarios represent the combination (if applicable) of exposure pathways for an individual based on his/her activity patterns.

4.2.3 Quantification of Exposure

Although exposure concentrations are based on the measured environmental concentrations for both current and future land use considerations, they often display variability between different sites within a watershed. It is important to understand that medium- and site-specific considerations influence the derivation of the exposure concentration. These considerations include the size of the site, land use designation, techniques used for data aggregation, and selection of applicable spatial statistics. Detailed guidance for determining the area of exposure units, exposure concentrations, and related issues is provided in Appendix G.

It should be noted that fate and transport modeling may be required to estimate exposure concentrations in the future. The project team should determine if fate and transport modeling would benefit the overall project and the associated risk assessment. Potential site-specific modeling decisions should be made in association with Data Quality Objective (DQO) decisions to ensure that models will be supplemented by sampling data and effectively support risk assessment activities. Appendices D-F provide guidelines on air dispersion modeling, groundwater modeling, and food chain models for use in risk assessment.

Exposure concentrations serve as one input variable in the equations that are used to calculate pathway-specific intakes for each receptor. As previously mentioned, many of the exposure equations that support the land uses on the ORR and at Paducah and Portsmouth are available on the RAIS along with default parameter values. These equations are updated as new technical information becomes available.

4.3 TOXICITY ASSESSMENT

The purpose of a toxicity assessment is to weigh available evidence regarding the potential for a chemical to cause adverse effects in exposed individuals and to provide, where possible, an estimate of the relationship between the extent of exposure and the increased likelihood and/or severity of adverse effects. (EPA 1989) Toxicity values for carcinogenic and noncarcinogenic chemicals and radionuclides are available for use by all subcontractors performing work for the DOE-ORO via the RAIS. Toxicity profiles for a select set of chemicals are also available via the RAIS.

4.3.1 Toxicity Values

A database of chemical-specific toxicity values is maintained on the RAIS. The toxicity values database contains information obtained from the EPA's Integrated Risk Information System (IRIS), the Health Effects Assessment Summary Tables (HEAST), and other information sources; all information contained in the database is referenced. In addition, the database contains supplemental information clarifying some issues.

The toxicity values contained in the RAIS database were developed for human health risk evaluations and assessments utilizing methods presented in part A of *Risk Assessment Guidance for Superfund: Volume 1-Human Health Evaluation Manual* (EPA 1989). The toxicity values database contains footnoted entries for toxicity values that have been withdrawn from IRIS, are provisional, or have been derived from other information. These footnoted values have been approved (by EPA Region IV) for use in the risk assessment and evaluation of areas on the ORR and Paducah. In addition, the

database incorporates information not considered in EPA's *Soil Screening Guidance* (i.e., dermal toxicity values and radionuclide toxicity values).

4.3.2 Toxicity Profiles

A database of toxicity profiles was developed using information from the EPA's IRIS and HEAST and other literature sources. The profiles and their references are provided on the RAIS to eliminate duplication of effort and to supplement the human health risk-based PRGs presented elsewhere on the RAIS.

In the toxicity profiles database, the profiles are presented in two formats:

- **Formal format**: Profiles are several pages long and are similar to the profiles found in IRIS; they are available for downloading in WordPerfect format.

- **Condensed format**: Profiles are generally less than a page in length and are suitable for use as a toxicity profile in the toxicity assessment chapter of a human health risk assessment.

4.4 RISK CHARACTERIZATION

The risk characterization section of a risk assessment incorporates the outcome of the previous activities (i.e., data evaluation, exposure assessment, and toxicity assessment) and calculates the risk or hazard resulting from potential exposure to chemicals via the pathways and routes of exposure determined appropriate for the site. Risk characterization integrates and summarizes the information presented in the exposure and toxicity assessments for each of the different land use scenarios in light of the associated uncertainties.

When characterizing risk, the risk assessor may decide to aggregate the data (e.g., based on depth, location, etc.) or compare risks on a point-by-point basis. Often the point assessment is a screening step for hot spots, chemicals of concern (COCs), etc. The aggregate assessment, based on the appropriate exposure scenarios, is typically the basis for remediation.

The following equations were taken directly from part A of the *Risk Assessment Guidance for Superfund: Volume 1-Human Health Evaluation Manual* (EPA 1989). Equation 1 is a numeric estimate of the systemic toxicity potential posed by a single chemical within a single route of exposure. Equation 2 is a numeric estimate of the systemic toxicity potential posed by all chemicals reaching a receptor through a single exposure route. Equation 3 is a numeric estimate of the systemic toxicity potential posed to a receptor by exposure to all chemicals over all routes. This last value is often called an estimate of "total noncarcinogenic risk".

The result of Equation 4 is an estimate of the increased cancer incidence (i.e., probability) to a receptor that results from exposure to a single chemical (or radionuclide) within a single exposure route. The result of Equation 5 is an estimate of the increased cancer incidence (i.e., probability) that results from exposure to all chemicals (or radionuclides) reaching a receptor through a single route. Finally, the result of Equation 6 is an estimate of the increased cancer incidence (i.e., probability) that results from exposure to all chemicals (or radionuclides) reaching a receptor over all routes. This last value is often called an estimate of "total carcinogenic risk".

Equation 1. A single chemical within a single exposure route:

$$HQ_i = \frac{CDI_i}{RfD_i}$$

where: HQ_i = The hazard quotient, an estimate of the systemic toxicity posed by a single chemical.
CDI_i = The estimate of chronic daily intake (or absorbed dose for some exposure routes) from the exposure assessment.
RfD_i = The chronic reference dose for administered or absorbed dose, as appropriate.

Equation 2. All chemicals within a single exposure route:

$$HI_p = \sum_{i=1}^{n} HQ_i$$

where: HI_p = The pathway hazard index, an estimate of the systemic toxicity posed by all chemicals within a single exposure route.
HQ_i = The individual chemical hazard quotients for chemicals reaching the receptor through a single exposure route (from Eq.1).

Equation 3. All chemicals over all exposure routes:

$$HI_{total} = \sum_{p=1}^{n} HI_p$$

where: HI_{total} = The total hazard index, an estimate of the systemic toxicity posed by all chemicals over all routes.
HI_p = The pathway hazard indices from Eq.2

Equation 4. A single chemical within a single exposure route:

$$ELCR_i = CDI_i \times SF_i$$

where: $ELCR_i$ = The chemical-specific excess cancer incidence.
CDI_I = The estimate of chronic daily intake (or absorbed dose) from the exposure assessment.
SF_i = The slope factor for administered or absorbed dose.

Equation 5. All chemicals within a single exposure route:

$$ELCR_p = \sum_{i=1}^{n} ELCR_i$$

where: $ELCR_p$ = The pathway-specific excess cancer incidence.
$ELCR_i$ = The chemical-specific excess cancer incidence from Eq. 4.

Equation 6. All chemicals over all exposure routes:

$$ELCR_{total} = \sum_{p=1}^{n} ELCR_p$$

where: $ELCR_{total}$ = The total excess cancer incidence posed by all chemicals over all routes.
$ELCR_p$ = The pathway-specific excess cancer incidence.

4.4.1 Selecting Scenarios, Pathways, and Chemicals of Concern (COCs)

The selection of scenarios, pathways, and COCs follows the guidelines outlined by the EPA Region IV in *Office of Technical Services Supplemental Guidance to RAGS: Region 4 Bulletins* (EPA 1996). These guidelines are outlined below.

Scenarios of Concern. Total noncarcinogenic risk (HI_{total}) and total carcinogenic risk ($ELCR_{total}$) will be compared to 1.0 and 1 x 10^{-4}, respectively, within a use (land use) scenario. Use scenarios with an overall cumulative HI_{total} or $ELCR_{total}$ exceeding either of these limits will be deemed "use scenarios of concern".

Pathways of Concern. Risk characterization results for excess lifetime cancer risks ($ELCR_p$) and hazard indices (HI_p) for routes over all COPCs within *a use scenario of concern* will be compared to 0.1 and 1 x 10^{-6}, respectively. Routes within *a use scenario of concern* exceeding either of these limits will be deemed "pathways of concern" for the use scenario of concern.

Chemicals of Concern. Results for excess lifetime cancer risk ($ELCR_i$) and hazard quotient (HQ_i) for COPCs over all routes within a *use scenario of concern* will be compared to limits of 0.1 and 1 x 10^{-6} respectively. COPCs within *a use scenario of concern* exceeding either of these limits will be deemed COCs for the use scenario of concern.

Media of Concern. For each pathway of concern, the $ELCR_{total}$ and HI_{total} for each medium within that pathway will be compared to 0.1 and $1x10^{-6}$, respectively. Media of concern will be those media that exceed these limits.

4.4.2 Verification of Calculations

Before the D1 version of any risk assessment is final, results of all risk/hazard calculations, including developed PRGs, should be independently verified. Risk assessors should implement "Verification of Human Health and Ecological Risk Assessments" (EMEF/EM-P2009) or an equivalent procedure. Documentation to support this verification should be included with the project files.

4.4.3 Presenting the Risk Characterization Results

In January 1998, the EPA issued *Risk Assessment Guidance for Superfund: Volume I, Human Health Evaluation Manual (Part D, Standardized Planning, Reporting, and Review of Superfund Risk Assessments)* (EPA 1998). As the title suggests, RAGS Part D provides guidance on standardized risk assessment planning, reporting, and review throughout the CERCLA remedial process, from scoping through remedy selection and completion and periodic review of the remedial action. The application of this standardized methodology on the ORR is a subject of much debate. Further guidance on the use of these standardized tables and reporting criteria will be provided by the Bechtel Jacobs Company LLC Risk Compliance and Reduction Program as it becomes available. For now, risk assessment results must provide all of the pertinent information necessary for making a remedial decision regarding risks/hazards.

4.5 UNCERTAINTY ANALYSIS

Estimation of uncertainty is fundamental to activities that involve measured or assessed quantities. Over- or under-estimates can lead to improper remedial decisions. Since the risk estimates generated in a risk assessment are based on exposure and toxicity assumptions, it is necessary to specify the assumptions and uncertainties in the risk assessment report. Specifically, uncertainties should be interpreted relative to their impact on risks and consequently remediation in the characterization section of the risk assessment report. Uncertainties may be present in selection of COCs, dose-response relationships, etc. For guidance on conducting an uncertainty analysis, refer to Appendix H of this document or *An Introductory Guide to Uncertainty Analysis in Environmental and Health Risk Assessment* (ES/ER/TM-35/R1).

5. SCREENING RISK ASSESSMENTS

Human health screening risk analyses, as presented in this document, include comparing available environmental data with risk-based Preliminary Remediation Goals (PRGs) and developing/updating an integration point assessment. These analyses were developed to accelerate the remedial investigation process and reduce its cost by identifying sources that are of highest priority. Since their development, the screening risk assessments have been applied to other projects [e.g., Decontamination and Decommissioning (D&D) and reindustrialization] to identify the potential risks and the need for risk reduction prior to the demolition or reuse of a facility. The screening risk analyses also identify and provide justification for early actions at sites. Lastly, these assessments can be used to focus data collection efforts on chemicals of potential concern or to identify data needs.

The screening risk assessments described in this document were based on the known physiographic, hydrologic, and geographic characteristics of the Oak Ridge Reservation (ORR) and existing/historical chemical environmental data. This information indicated that the surface water and groundwater systems on the ORR serve as collectors or basins for multiple chemicals from a variety of sites. These chemicals are mixed together within these water bodies and integrated into their flow system. As such, the surface water and groundwater systems are referred to as integrators. Most importantly, these integrators, along with the air pathway, are the primary means of contaminant transport to areas outside the boundaries of the ORR where public exposure becomes more probable. A screening risk analysis methodology, called the integration point assessment, was developed to evaluate the surface water integrators.

The integration point assessment is a flux-based risk assessment method developed to evaluate the surface water integrators. This assessment uses monitoring, surveillance, compliance, and other data to evaluate relative contribution to the off-site risk from the various input sources of surface water integrators. Once the primary sources in the integrator are identified, source control actions can be prioritized and undertaken to reduce exposure to levels that are as low as reasonably achievable.

The combination of the comparison to risk-based PRGs and the integration point assessment allow the risk manager to prioritize sites relative to both on-site and off-site risk/hazard [where “site” refers to the U.S. Department of Energy (DOE) ORR property], respectively. These assessments can be performed at any point during the investigative process and can be updated as new information becomes available.

5.1 COMPARISON TO RISK-BASED PRELIMINARY REMEDIATION GOALS

Chemical-specific, risk-based PRGs, which are a subset of all PRGs, are concentration goals for individual chemicals and radionuclides for specific medium and land use combinations. The risk-based PRGs are derived using a specific excess lifetime cancer risk or hazard index. Risk-based PRGs are initial guidelines that are protective of human health and the environment, based on readily available information, and comply with Applicable or Relevant and Appropriate Requirements (ARARs). For more information on PRGs, refer to Section 1.1 of *Risk Assessment Guidance for Superfund, Part B* (EPA 1991a).

The Risk Assessment Information System (RAIS) provides the means to calculate risk-based PRGs using standard exposure equations for a number of exposure routes. This interactive web program allows the user to select analytes of interest and to customize the exposure equations for the routes they wish to evaluate. For more information please see the web page at: http://www.risk.lsd.ornl.gov/rap_prg.

The guidelines in this document dictate the use of the risk-based preliminary remediation goal screening assessment during data evaluation activities to aid in identifying:

- chemicals of potential concern,
- transport and exposure pathways that need to be further characterized,
- data gaps and limitations,
- appropriate detection limits for subsequent sampling efforts,
- high priority on-site areas, and
- sites for which a no further investigation/action determination may be appropriate.

5.1.1 Risk-Based Preliminary Remediation Goal Screening to Determine Chemicals of Potential Concern in the Baseline Human Health Risk Assessment

A screening using chemical-specific, risk-based PRGs will be conducted during data evaluation of the baseline human health risk assessment as part of the identification of chemicals of potential concern (COPCs). Analytes detected above background (when available) for each exposure pathway are compared to chemical-specific, risk-based PRGs for the residential scenario. The pathways that have been identified to be included in the risk assessment are those deemed necessary to support project Data Quality Objectives (DQOs) (e.g., remedial decisions). It should be noted that analytes whose maximum detected concentrations are less than the chemical-specific risk-based PRGs (i.e., $ELCR_i \leq$ 1E-06 or $HQ_i \leq 0.1$ or if $ECLR_i \leq$ 1E-06 and $HQ_i \leq 0.1$) for the residential scenario do not significantly contribute to the $ELCR_{total}$ and/or HI_{total} and therefore may be eliminated from the quantitative risk assessment.

In addition, if no analyte in the site, land use scenario, or pathways exceeds the most conservative preliminary remediation goal, any or all of the sites, land uses scenarios, or pathways may be designated no action (i.e., the preliminary remediation goal screen is sufficient to support no action).

5.1.2 Risk-Based Preliminary Remediation Goal Screening to Support Characterization Activities

In addition to the selection of COPCs, risk-based PRG screening can support site characterization activities. The screening of existing/historical data against the risk-based PRGs for the exposure pathways being evaluated in the risk assessment can:

- identify data needs and limitations,
- focus future sampling and analysis on chemicals and exposure pathways of concern, and
- establish appropriate detection limits for subsequent sampling and analysis activities.

5.1.3 Risk-Based Preliminary Remediation Goal Comparison for Identifying High Priority On-site Areas

The identification of high priority on-site areas (e.g., within a large watershed) may be accomplished by a comparison with risk-based PRGs. Values representing current time/activity patterns may be used, if available. Extensive research to develop site-specific exposure parameters is neither required nor recommended prior to completing this comparison. The Risk Assessment Technical Lead (RATL) must use all available information and best professional judgement to derive exposure scenarios and parameters representative of current conditions. The Risk Advisory Board (RAB) must approve these parameters prior to their use.

The purpose of this screening is not to determine actual/current exposure at the sites but to simply identify those source areas that pose the highest risk (i.e., they fail the screening). A removal action or some other type of early response action may be necessary if the chemicals are present, accessible, and

fail the screening. If the chemicals present at a site pass this screening, it is simply an indication that further assessment should be conducted to determine the need for continued investigation.

5.2 INTEGRATION POINT ASSESSMENTS

For the ORR sites, the majority of any off-site public exposure to chemicals of potential concern results from exposure to contaminants in surface water because surface water is the primary receiving medium in and around the reservation. Other potential receiving media, such as agricultural products, air, and groundwater, are currently not primary exposure media. The integration point assessment, which supports watershed actions, is designed to actively use monitoring, surveillance, compliance, and Remedial Investigation (RI) data to evaluate off-site risk from a variety of sources that input into the surface water integrator. The data will be used to:

- establish a baseline for evaluating the risk at different points within the integrators;
- identify and prioritize sites within the context of the integrator; and
- estimate the potential risk reduction resulting from an action to control contaminant sources.

Note: The integration point assessment provides critical information to the baseline human health risk assessment because of frequent updates (as data become available). As the integration point assessment is updated, the results are used to provide current estimates of potential risk/hazard at the surface water or watershed level.

The integration point assessment is a flux-based screening assessment. Flux is defined as the mass of chemical that migrates through a cross-sectional area in a given time. Flux is important because of the number of actual and potential sources of chemicals that exist on the ORR. In addition, there is considerable variability in flow rates of the different surface water systems that transport these chemicals to the surface water integrator sites and eventually to the Clinch River (near the ORR). Controlling sources of contamination at areas with high fluxes of integrator chemical of concern (COCs) is the quickest means of reducing contaminant concentrations in off-site areas to target levels.

One of the more important objectives during early phases of an integrator site investigation is to assimilate available information from existing programs to estimate fluxes and mass balances of chemicals within the integrator system. The information is then used to assess fluxes within the watershed and compare them to fluxes that input into public access areas in order to differentiate between various contaminant sources at the ORR. Mass balance information is important for describing the accumulation and discharge of chemicals within a system where inputs and outputs are known. The integration point assessment allows communication of this information in terms of risk to the public and risk managers. It also provides an important link between the risk posed by contamination at source locations and risk posed by contamination in surface water integrators so that the impact of actions to control contaminant fluxes at sources can be evaluated at the integrator or watershed level. Appendix I provides a detailed description of the integration point assessment methods.

6. BASELINE HUMAN HEALTH RISK ASSESSMENTS

The baseline human health risk assessment (BHHRA) is an analysis of the potential adverse health effects caused by exposure to hazardous substances released from a site in the absence of any actions to control or mitigate these releases (i.e., under an assumption of no action). The BHHRA contributes to the characterization and subsequent development, evaluation, and selection of appropriate response alternatives. The results of this assessment are used in the feasibility study to:

- document the magnitude of risk/hazard at a site identify the chemicals of concern,
- establish remedial goal options (i.e., clean-up levels),
- finalize the remedial action objectives, and
- help support the selection of the "no action" remedial alternative, where appropriate.

A baseline human health risk assessment will be performed for all sites and media within a watershed on the Oak Ridge Reservation (ORR) prior to final action. The exposure pathways and associated exposure parameters to be used in the BHHRA will depend on:

- the sources, releases, types, and locations of chemicals at the site;
- the likely environmental fate of the chemicals;
- the proposed future use of the site (i.e., land use or end use); and
- the potentially exposed populations.

As previously mentioned, the BHHRA process on the ORR will follow the regulatory guidance outlined in Table 4. In addition, the guidelines contained in this document are provided to ensure that all human health risk assessments and related risk activities for the U.S. Department of Energy, Oak Ridge Operations (DOE-ORO) Environmental Management (EM) Program are consistent with both program and regulatory guidance and are technically defensible.

7. RISK ASSESSMENT IN AND AFTER THE FEASIBILITY STUDY

The feasibility study is a two-step process consisting of a preliminary screening of alternatives [(usually based on the identification of chemicals of potential concern (COPCs) and performed prior to the final completion of the baseline human health risk assessment (BHHRA)] and a detailed analysis of those alternatives that pass the initial screening. Once the BHHRA is completed and a list of chemicals of concern is available, a more thorough screening of alternatives may be completed prior to the detailed analysis of alternatives to further reduce the number of alternatives evaluated in the feasibility study.

The focus of the BHHRA is to evaluate the effect of selecting a "no-action" alternative on human health. The focus of the feasibility study is to evaluate both the short-term and long-term risks associated with the actual implementation of a remedial alternative (see Table 3). Short-term risks associated with a remedial alternative are those risks that occur during the implementation of the alternative (e.g., risks from emissions) and affect the persons who live and work near the site and the actual workers who are performing site remediation. Long-term risks are those risks that will remain after the remedy is complete (i.e., residual risk either from treatment residuals or untreated waste). In addition, the evaluation of long-term risks considers the effectiveness of the remedy over time.

The methods for assessing both short-tem and long-term risks are the same as those for the BHHRA. The major differences are

- the estimation of timing and duration of exposures,
- the estimation of source terms (i.e., concentrations) to be evaluated at various times over the course of the remedy,
- the need for short-term toxicity values (i.e., chronic values may need to be modified since the exposure duration will be less than a lifetime), and
- the consideration of worker risks including health and safety issues.

Risk evaluations subsequent to the feasibility study are conducted on an "as needed" basis to ensure that the remedy is and continues to be protective. If new environmental data or other information that would serve to refine previous analyses becomes available after the feasibility study is complete, this information, and its effects on all proposed alternatives, is incorporated into the Proposed Remedial Action Plan.

The Record of Decision includes a section on comparative analysis that discusses risk as it pertains to long-term effectiveness, short-term effectiveness, and overall protection of human health and the environment. This section also discusses how the remedy will eliminate, reduce, or control the risks identified in the baseline human health risk assessment; whether or not the remedy meets the established remedial goal options; and any risks resulting from residual materials.

Note: Remedial Goal Options (RGOs) are chemical-specific. Medium-specific, numerical concentration limits that are identified for all contaminants and all pathways found to be of concern during the BHHRA. RGOs are not the first or the final set of cleanup levels in the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) process but can be viewed as modified Preliminary Remediation Goals (PRGs) based on site characterization and risk assessment findings. RGOs are valuable for designing Data Quality Objectives (DQOs) in the Remedial Investigation process, for comparison to detected contaminant concentrations, and as criteria in selecting and designing remediation alternatives in the Feasibility Study.

The evaluation of risks during the remedial design/remedial action phase of a project may be limited to the continued evaluation of short-term and long-term risks if no new contaminant information is discovered. Monitoring data is collected during the implementation of the remedial alternative to address the short-term risks to the public and workers. In addition, sampling to determine whether or not a remedy has attained the appropriate clean-up levels is conducted. The risk assessor is integral to the development of each sampling and analysis plan because residual risks for the chemicals of concern must be determined to demonstrate successful completion of the remedy. Such an evaluation of the residual risk at that time is useful during the five-year review, especially if new environmental data become available.

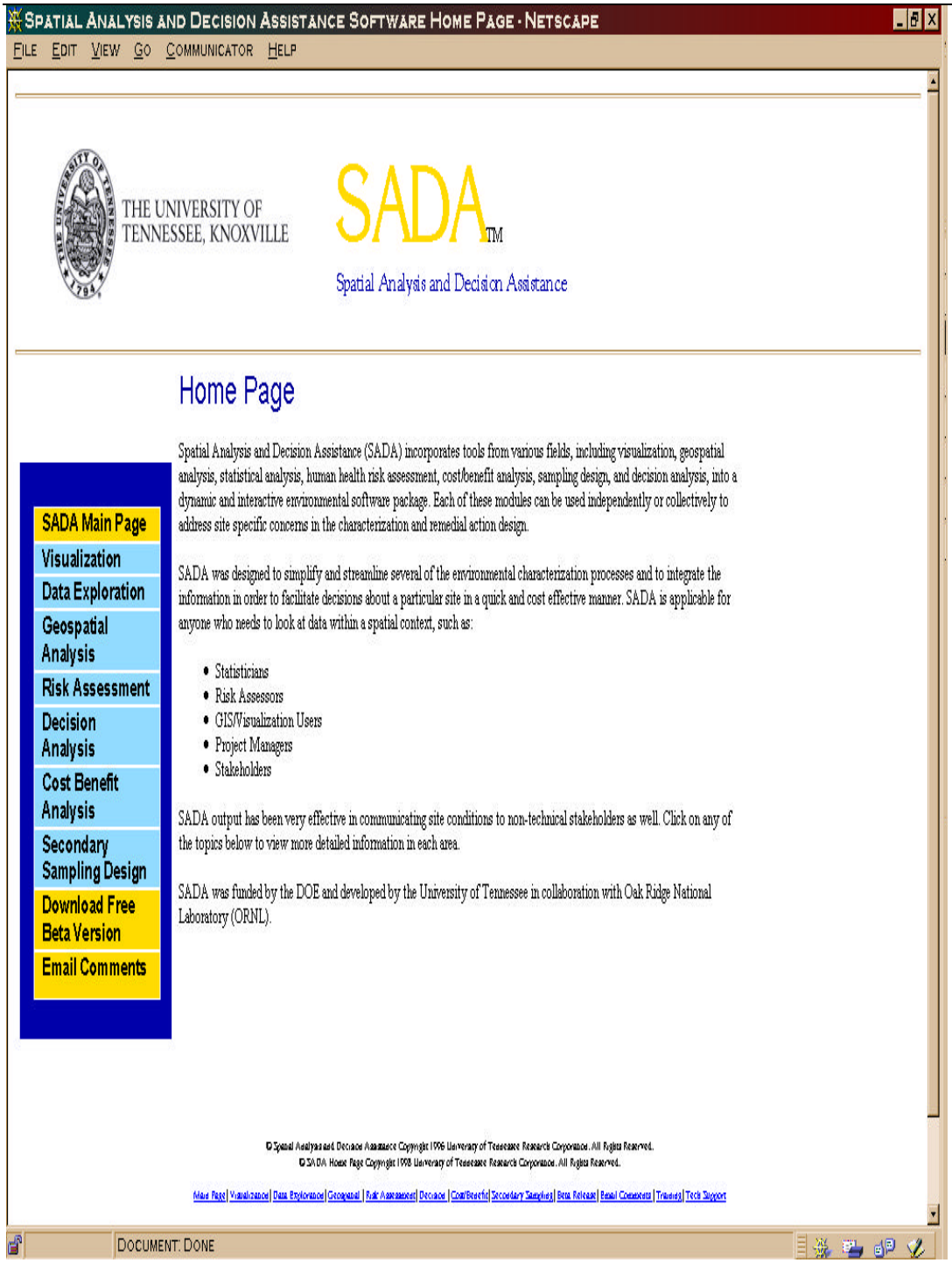
If new toxicity or other data become available at the time of the five-year review, the results of the baseline risk assessment may need revision. A decision to revise the baseline as part of the five-year review is made by the risk managers (i.e., EPA, TDEC, and DOE-ORO).

Guidance on conducting a feasibility study can be found in the EPA document *Guidance for Conducting Remedial Investigations and Feasibility Studies Under CERCLA* (EPA 1988). Risk assessment in the feasibility study is discussed in detail in *Risk Assessment Guidance for Superfund Vol. I - Part C, Risk Evaluation of Remedial Alternatives* (EPA 1991b).

8. RISK ASSESSMENT INFORMATION SYSTEM

In order to provide a ready source of information needed to complete environmental risk assessments for the Department of Energy, Oak Ridge Operations (DOE-ORO), the DOE Center for Risk Excellence (CRE) and the DOE-ORO sponsor a web-based system that contains risk tools and other information. This system, the Risk Assessment Information System (RAIS), was developed to support site-specific needs of the former DOE-ORO Environmental Restoration Risk Assessment Program. With support from the CRE, the system is being expanded and reconfigured to benefit all DOE risk information users and the risk community. With searchable and executable databases, menu-driven queries, and data downloads, the RAIS offers essential tools that are used in the risk assessment process from project scoping to implementation. A training course for the RAIS will be held late summer 1999. The RAIS may be found at http://risk.lsd.ornl.gov/.

Spatial Anaysis and Decision Assistnace (SADA) software was designed to simplify and streamline the environmental characterization process and to integrate the information in order to facilitate decisions about a particular site in a quick and cost-effective manner. SADA was funded by the DOE and developed by the University of Tennessee in collaboration with the Oak Ridge National Laboratory. To obtain more information about SADA and its upcoming training course or to download a free version of the software, go to http://www.sis.utk.edu/cis/sada/.



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APPENDIX A

RISK ASSESSMENT TECHNICAL MEMORANDA

BJC/OR-55 *Guidance for Treatment and Variability and Uncertainty in Ecological Risk Assessments of Contaminated Sites* (formerly ES/ER/TM-228)

This report offers guidance for the analysis and presentation of variability and uncertainty in ecological risk assessments. This report discusses concepts of probability in terms of variance and uncertainty, describes how these concepts differ in ecological risk assessment and human health risk assessment, and describes probabilistic aspects of specific ecological risk assessment techniques.

BJC/OR-80 *Radiological Benchmarks for Screening Contaminants of Potential Concern for Effects on Aquatic Biota at Oak Ridge National Laboratory, Oak Ridge, Tennessee* (formerly ES/ER/TM-226)

The radiological benchmarks in this report are to be used at the U.S. Department of Energy's (DOE) Oak Ridge Reservation (ORR) and at the Portsmouth and Paducah gaseous diffusion plants as screening values only to show the nature and extent of contamination and identify the need for additional site-specific investigation. The screening values presented in this document include internal and external exposures from parent isotopes and all short-lived daughter products.

BJC/OR-112 *Biota-Sediment Accumulation Factors for Invertebrates: Review and Recommendations for the Oak Ridge Reservation*

This report acquires contaminant uptake data from published and unpublished literature, develops and presents biota-sediment accumulation factors and regression equations for estimating chemical concentrations in benthic invertebrates for use on the ORR, and compares these to contaminant uptake data for emergent adult insects. The equations and accumulation factors presented in this report facilitate the estimation of contaminant exposure experienced by wildlife consuming flying insects on the ORR.

BJC/OR-133 *Empirical Models for the Uptake of Inorganic Chemicals from Soil by Plants*

This report develops soil-plant contaminant uptake models using published data from soil contamination in the field and validates the models using measured concentrations from two contaminated sites. This report provides a means to estimate concentrations of the inorganic chemicals in aboveground plant biomass, if only concentrations in soil are measured.

BJC/OR-157 *An Investigation of, and Recommendations for, Statistical Comparisons Between Site and Background, Both With and Without Censoring* (DRAFT)

This report provides an evaluation of numerous statistical methods that may be applied in order to determine whether sites are contaminated. This analysis relies primarily on statistical considerations and on results of extensive computer simulations that provide comparisons of the statistical tests under conditions that are expected to apply when contamination exists and when it does not.

ES/ER/TM-28 *The Use of Institutional Controls at Department of Energy Oak Ridge Field Office Environmental Restoration Sites*

This report summarizes major issues related to the use of institutional controls at hazardous waste sites under the auspices of the DOE-OR/Environmental Restoration (ER) Division. In particular, the report addresses the impacts that assumptions regarding institutional controls have on the results and interpretations of risk assessment in the Remedial Investigation/Feasibility Study.

ES/ER/TM-33/R2 *An Approach and Strategy for Performing Ecological Risk Assessments for the U.S. Department of Energy's Oak Ridge Reservation: 1995 Revision*

This report provides specific guidance for planning and performing ecological risk assessments on the ORR and promotes the use of consistent approaches. Although developed for the ORR, this strategy may be applicable to other complex Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) sites that possess significant ecological resources.

ES/ER/TM-35/R1 *An Introductory Guide to Uncertainty Analysis in Environmental and Health Risk Assessment*

This report presents guidelines for evaluating uncertainty in mathematical equations and computer models applied to assess human health and environmental risk. The subjective confidence levels from an uncertainty analysis should produce a reasonably "high" probability of bounding the true risk, provided that risk assessors avoid overconfidence in quantifying the level of certainty associated with important model components.

ES/ER/TM-38 *Approach and Strategy for Developing Human Health Toxicity Information for Contaminants of Concern at Sites Administered by the U.S. Department of Energy Oak Ridge Field Office Environmental Restoration Program*

This report develops toxicity values for chemicals of concern (COCs) at DOE-ORO sites for which no EPA-approved values have previously been developed. With dose and toxicity estimates for all COCs, a quantitative approach to assessing risks to human health can be made.

ES/ER/TM-78 *Methodology for Estimating Radiation Dose Rates to Freshwater Biota Exposed to Radionuclides in the Environment*

This report presents a methodology for evaluating the potential for aquatic biota to incur effects from exposure to chronic low-level radiation in the environment. Previously developed dose rate equations are presented for estimating the radiation dose rate to representative aquatic organisms from alpha, beta, and gamma irradiation from external and internal sources.

ES/ER/TM-85/R3 *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Terrestrial Plants: 1997 Version*

This technical memorandum presents plant toxicity data and discusses their utility as benchmarks for determining the hazard to terrestrial plants caused by

contaminants in soil. The report provides a standard method for deriving benchmarks, a set of data concerning the effects of chemicals in soil or soil solution on plants, and a set of phytotoxicity benchmarks for 38 chemicals potentially associated with United States DOE sites.

ES/ER/TM-86/R3 *Toxicological Benchmarks for Wildlife: 1996 Revision*

This report presents toxicological benchmarks to assess the effects of certain chemicals on mammalian and avian wildlife species. The document provides toxicological benchmarks that may be used as comparative tools in screening assessments as well as lines of evidence to support or refute the presence of ecological effects in ecological risk assessments.

ES/ER/TM-95/R4 *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Sediment-Associated Biota: 1997 Revision*

This report presents sediment benchmark data and discusses their use as benchmarks for determining the level of toxicological effects on sediment-associated biota and describes three categories of approaches to the development of sediment quality benchmarks. It contains new benchmarks for freshwater sediments, equilibrium partitioning benchmarks corrected to two significant figures, and all of the freshwater and estuarine benchmarks included in the previous version.

ES/ER/TM-96/R2 *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Aquatic Biota: 1996 Revision*

This report presents and analyzes alternate toxicological benchmarks for screening chemicals for aquatic ecological effects. The alternate benchmarks are based on different conceptual approaches to estimating concentrations that cause significant effects.

ES/ER/TM-112/R2 *Environmental Restoration Risk-Based Prioritization*

The methodology discussed in this report was developed to evaluate and rank ER work packages on the basis of overall value (e.g., risk reduction, stakeholder confidence) to ER. This document presents the technical basis for the decision support tools and prioritization process.

ES/ER/TM-117/R1 *Risk Assessment Quality Program Plan*

This document specifies quality assurance requirements and applicable standards and procedures for risk assessment. This document provides a plan that identifies the responsibilities of Risk Assessment Program personnel and the chain of command for executing quality requirements.

ES/ER/TM-125 *Estimating Exposure of Terrestrial Wildlife to Contaminants*

This report describes generalized models for the estimation of contaminant exposure experienced by wildlife on the ORR. Because wildlife are mobile and generally consume diverse diets and because environmental contamination is not

spatially homogeneous, factors to account for variation in diet, movement, and contaminant distribution have been incorporated into the models.

ES/ER/TM-126/R2 *Toxicological Benchmarks for contaminants of Potential Concern for Effects on Soil and Litter Invertebrates and Heterotrophic Process: 1997 Revision*

This report presents a standard method for deriving benchmarks for the purpose of "contaminant screening", which is performed by comparing measured ambient concentrations of chemicals. In addition, this report presents sets of data concerning the effects of chemicals in soil on invertebrates and soil microbial processes, benchmarks for chemicals potentially associated with DOE sites, and literature describing the experiments from which data were drawn for benchmark derivation.

ES/ER/TM-131 *Radiological Criteria for Remedial Actions at Radioactively Contaminated Sites*

This report presents radiological criteria for determining acceptable remedial actions at radioactively contaminated sites on the ORR. This report also describes two different approaches to risk management under the Atomic Energy Act and CERCLA and demonstrates how the proposed remedial action criteria can be reconciled with the requirements of CERCLA.

ES/ER/TM-134 *Decision Support for CERCLA Investigations: An Introduction to Decision Analysis Applications*

This report provides the Oak Ridge Operations (ORO) Environmental Restoration (ER) technical community with an introduction to various decision analysis applications and their relevance to the CERCLA process. The long-term goal of investigating the decision analysis literature is to find specific applications that are useful in the collection of data and the selection of alternatives.

ES/ER/TM-146 *Geostatistical Applications in Environmental Remediation*

This report defines the advantages and limitations of geostatistical analysis and demonstrates how it may be effectively used in environmental problems. Geostatistics provide human health and ecological risk assessors with a powerful tool that can better delineate the spatial distribution and uncertainty of risk calculations than traditional methods.

ES/ER/TM-153 *Guide for Performing Screening Ecological Risk Assessments at DOE Facilities*

This report provides guidance for performing screening ecological risk assessments, which are a major component of the RI process. Use of this guidance document will standardize the methodology used in preparing screening ecological risk assessments and will narrow the scope of subsequent assessment activities by focusing on those aspects of the hazard that constitute credible potential risks.

ES/ER/TM-162/R2 *Preliminary Remediation Goals for Ecological Endpoints*

This report presents Preliminary Remediation Goals (PRGs) for ecological endpoints used for risk assessments and decision making at CERCLA sites. Preliminary Remediation Goals are upper concentration limits for specific chemicals in specific environmental media that are anticipated to protect human health or the environment. They can be used for multiple remedial investigations at multiple facilities.

ES/ER/TM-165 *D&D Screening Risk Evaluation Guidance*

The screening risk evaluation provides a semi-quantitative program-level screening of facilities. Its intent is to provide a quick and efficient means of evaluating current and future risks from Decontamination and Decommissioning (D&D) facilities using existing historical, process, occurrence, monitoring, and compliance data. This document provides guidance for conducting a screening risk evaluation for D&D facilities.

ES/ER/TM-185/R1 *Guide for Developing Data Quality Objectives for Ecological Risk Assessment at DOE Oak Ridge Operations Facilities*

This report presents guidance for developing data quality objectives for ecological risk assessment performed as components of the RI process. Use of this guidance document will standardize the methodology used in developing data quality objectives for ecological risk assessments and will narrow the scope of subsequent data collection and risk assessment activities by focusing on those aspects of the hazard that are most relevant to decision making.

ES/ER/TM-186 *Guide for Developing Conceptual Models for Ecological Risk Assessment*

This report presents guidance for preparing conceptual models for ecological risk assessments. Use of this guidance document will standardize the conceptual models used in ecological risk assessment so that they will be of high quality, useful to the assessment process, and sufficiently consistent so that connections between sources of exposure and receptors can be extended across operable units.

ES/ER/TM-187 *Criteria for Establishing De Minimis Levels of Radionuclides and Hazardous Chemicals in the Environment*

This report develops proposed criteria for establishing *de minimis* levels of radionuclides and hazardous chemicals in the environment. The proposed criteria are consistent with objectives for remediation of contaminated sites under CERCLA, additional regulatory guidance for implementing the CERCLA remediation objectives, and various other regulatory precedents and recommendations.

ES/ER/TM-200 *Risk Characterization for Ecological Risk Assessment of Contaminated Sites*

This document describes an approach for estimating risks based on individual lines of evidence and then combining them through a process of weighing the evidence. This document expands the risk characterization guidance from

ES/ER/TM-33/R2 by providing more specific information on how ecological risk characterization should be performed.

ES/ER/TM-201 *Terrestrial Habitat Mapping of the Oak Ridge Reservation: 1996 Summary*

This report documents the work performed under the ORR-Wide Ecological Risk Assessment Program. It provides information on changes in land use and land cover between 1984 and 1994. This document also provides information on the potential spatial habitat distribution of two terrestrial species that may potentially be at risk from the effects of the operable units on the ORR.

ES/ER/TM-202 *Estimation of Whole-Fish Contaminant Concentrations from Fish Fillet Data*

This report presents the results of an investigation of the relationship between fillet and whole-fish contaminant concentrations and develops equations for the estimation of whole-fish concentrations for several analytes.

ES/ER/TM-210 *Ecological Profiles for Selected Metals and Other Inorganic Chemicals*

This technical memorandum presents profiles for chemicals of potential ecological concern. These profiles contain information concerning the relationship between exposure and response for the chemicals of potential ecological concern that are used to perform the risk characterization. Inclusion of these profiles in an assessment document will provide reviewers, stakeholders, and risk managers with the information needed to independently evaluate risk characterization.

ES/ER/TM-211 *Improved Methods for Calculating Concentrations Used in Exposure Assessments* (DRAFT)

This report will describe the computer programs that provide improved methods of determining the concentrations appropriate for use in ORO risk assessments. The ultimate objective of this report is to provide and explain new statistical software that should be applied to improve the concentration estimates.

ES/ER/TM-212 *Relative Risk Ranking Evaluation for the DOE Oak Ridge Operations*

This report provides relative risk ranking scores for sites under the auspices of the DOE-ORO. The information included in this report contains the list of release sites, the rank, the medium used to determine the rank, and the receptor.

ES/ER/TM-219 *Development and Validation of Bioaccumulation Models for Small Mammals*

This report documents the development of a database of soil and whole-body small mammal concentrations for 9 inorganic chemicals based on data from 22 studies from 4 countries and 9 states. This information will be used to evaluate risks to predatory wildlife on the ORR.

ES/ER/TM-220 *Development and Validation of Bioaccumulation Models for Small Mammals*

This report documents the development of a database of soil and tissue concentrations for 9 inorganic and 2 organic chemicals based on data from 31 studies from 11 countries and 5 states. This information will form a critical component in many ecological risk assessments performed on the ORR.

ES/ER/TM-223 *Parameters and Models for Estimation of Human Health Risks from Ingestion of Contaminated Game* (DRAFT)

The primary objective of this document is to provide the DOE-ORO with a standardized set of models and parameter values for estimating contaminant concentrations in human foods, specifically wild game. Provision of these models and recommended default values to contractors conducting risk assessments is meant to eliminate duplication of effort in model and parameter development.

ES/ER/TM-229 *Determination of the Spatial Risk to Wildlife from Dispersed Contaminants on the Oak Ridge Reservation, Oak Ridge, Tennessee* (DRAFT)

This report was prepared as a technical report documenting work performed under the ORR–Wide Ecological Risk Assessment Program. This document provides information on the potential spatial distribution of mercury contamination in soil as it relates to available short-tailed shrew habitat on the ORR.

ES/ER/TM-231 *Method for Calculating Preliminary Remediation Goals in Soil Protective of Groundwater* (DRAFT)

This report presents guidance for calculating PRGs in soils that are protective of groundwater for sites on the ORR. This report summarizes U.S. Environmental Protection Agency (EPA) guidance on methods for calculating safe levels of contamination that are protective of groundwater and gives default values for the ORR.

ES/ER/TM-232 *Risk Assessment Program Data Management Implementation Plan*

This document specifies data management requirements and applicable command media for the Risk Assessment Program. Specifically, this document provides guidance to control data receipt, processing, and use and discusses measures to ensure configuration control and access control to software changes.

Un-numbered *D&D Alternatives Risk Assessment* (DRAFT)

The D&D alternatives risk assessment supports the design and implementation of specific D&D alternatives by providing the risk assessment portion of the feasibility study or the streamline risk assessment for an engineering evaluation/cost analysis. Guidance for conducting an alternatives risk assessment is found in *Department of Energy - Oak Ridge Operations Environmental Management Program Risk Ranking Methodology*, (DRAFT) BJC/OR-127, Bechtel Jacobs Company, LLC, Oak Ridge, Tennessee.

K/ER-153/R1 *Baseline Risk Assessment Guidance for D&D Facilities*

The baseline risk assessment for D&D facilities is conducted in similar fashion to the baseline risk assessment for the RI. This document provides guidance for conducting a D&D baseline risk assessment that uses detailed characterization data to estimate potential current and future human health and environmental risks from the facility under investigation.

APPENDIX B

DATA EVALUATION

Sections B.1 through B.5 provided is this appendix outline the steps necessary to perform the data evaluation for human health risk assessments (HHRAs). These action steps are outlined sequentially.

B.1 REQUEST THE ANALYTICAL SAMPLING DATA

The risk assessor should make a verbal and written request for analytical sampling data to the Environmental Data Coordinator for the project (hereafter called the "data custodian"). The request should define the specific parameters that will be required for the data evaluation and state the specific electronic format that is desired; any deviations from the requested data structure should be cleared with the organization requesting the data/performing the risk assessment. A time frame for delivery of the data transmittal package should also be specified in this request. It should be noted that the majority of the existing environmental data for the Oak Ridge Reservation (ORR) is electronically available from the Oak Ridge Environmental Information System (OREIS).

In addition, the risk assessor should:

1. request that the data custodian verify that all of the data from the requested sampling event(s) are available in electronic format; if some data are missing or unavailable when they are transmitted, an explanation should be included along with the delivered data;

2. request that the data custodian provide a list of unique qualifiers that appear on the data set along with their definitions; and

3. inquire whether or not data validation has been performed on the data set and at what level (e.g., 100%, 10%, etc.), and if the data have not been 100% validated and quality control data (e.g., lab blanks) are available in the data set, then the five times and ten times rule for evaluation of blank samples must be performed.

B.2 RECEIVE AN ELECTRONIC COPY OF THE DATA

At a minimum, the data should be received in a tab-delimited ASCII file or a data base file that can be downloaded for data evaluation. Preferably, the data should be received in the requested format.

B.3 PERFORM QUALITY ASSURANCE/QUALITY CONTROL (QA/QC) ON THE DATA

This risk assessor should:

1. verify that all media for each area of potential concern in the investigation are included in the data set;

2. verify that all samples for each medium of potential concern for each area of potential concern are included in the data set;

3. verify that, where there is more than one area of potential concern, the data set includes identifiers that distinguish each medium of potential concern for each area of potential concern [this identifier will later assist in determining exactly where the sample was taken and in locating specific areas of high level of contamination (i.e., in hot spot identification) within an area of potential concern]; and

4. identify and correct any inconsistencies in the analytical data set using the following steps as a guide:

— Verify that units of measure for each medium of concern are reported consistently.

— Verify and revise the Chemical Abstract Service Registry Numbers (CASRNs) as necessary for each analyte in the data set; they must coincide with the CASRNs found on the Risk Assessment Information System (RAIS) (LMER 1998).

— Verify that the sample type is included in the data set. The type of sampling data (e.g., regular sample, field blank, trip blank, laboratory blank, duplicate, matrix spike, etc.) being reported must be indicated. The specific type of data (e.g., regular versus blank sample) should be identified by the laboratory performing the sample analysis. The data must be indicated as QC data or actual field sampling data (i.e., regular samples) obtained for those media of potential concern at the areas of potential concern that are being investigated. In addition, a mechanism must be in place for matching the original/regular samples with their associated duplicates, blanks, etc. (i.e., their QC data).

— Verify that analyte names are reported consistently in the analytical sampling data set [e.g., as listed on the RAIS (LMER 1998)]. The use of a different chemical name for the same analyte (e.g., trichloroethylene versus trichloroethene or cesium-137 versus Cs-137) would misrepresent the occurrence of that chemical in a data set. The most common chemical name should be used consistently throughout all data sets for the site evaluations to avoid confusion and error.

— Verify that the analytical method used by the laboratory is indicated (e.g., EPA method, American Society for Testing and Materials method, etc.) to determine the detection limit of the method used, and if the data will be acceptable for use in the HHRA. Although the detection limits should have been established as part of the data quality objectives (DQOs) process for suitability in risk assessments, sometimes a detection limit is greater than the risk-based Preliminary Remediation Goal (PRG); in this case, the analytical method should be evaluated and scrutinized against the acceptable uncertainties as defined in the DQOs process.

— Verify the sample quantitation limits of the analytical sampling techniques to determine whether the data are of acceptable quality for use in the HHRA. For example, an analytical technique with a high quantitation limit may be of limited value for use in a quantitative risk assessment.

— Conduct an evaluation of the laboratory data qualifiers and the data validation qualifiers. Various qualifiers are attached to the data by either the laboratory conducting the analyses or by individuals performing data validation. These qualifiers often pertain to QA/QC problems and generally indicate questions concerning chemical identity, chemical concentration, or both. Because the data validation process is intended to assess the effect of QC issues on data usability, validation data qualifiers are attached to the data after the laboratory qualifiers have been reported and, therefore, the validation qualifiers supersede the laboratory qualifiers. These data qualifiers are used to determine if the concentration is a detected concentration or not. All data designated with rejected data qualifiers (e.g., R) should not be included in the data evaluation for the HHRA unless justification is provided. All qualifiers must be addressed before the chemical can be used in a quantitative risk assessment.

— Verify the detection status for all radiological data. Information that should be used in the determination of detection status (e.g., detect, non-detect) includes all available qualifiers, reported concentrations, reported minimum detectable activities (MDAs), and reported uncertainties. As mentioned above, validation qualifiers supersede laboratory qualifiers. Decisions regarding how the reported concentrations, MDAs, and uncertainties are used to determine the detection status for radionuclides are usually made at the project level. For example, a project team may decide that after reviewing qualifiers, radionuclides must be further

evaluated by comparison to the reported concentrations, MDAs, and uncertainties. A possible decision may be that a radiological concentration is a detected concentration only if the reported concentration is greater than both the MDA and the uncertainty and that there are no qualifiers that suggest a non-detect status. The project team should establish criteria to address the situation where MDAs and/or uncertainties may not be available for radiological data, as well as how to handle negative concentrations (see discussion below).

— Evaluate negative concentrations. Negative concentrations or concentrations of zero (i.e., non-positive concentrations) are not expected for non-radionuclides. For these data, the risk assessor should consult with the data custodian about the accuracy of the concentrations. For radionuclides, however, non-positive concentrations can be legitimate since radiological data are often reported as the difference between a measured activity and the background activity. Several options are available for handling these non-positive radiological data, and this decision should be made on the project level. Three common options for evaluating non-positive radiological data are:

  - use a surrogate concentration of zero in all statistical calculations and set the detection status to non-detect for these data (this approach will generally increase the mean concentration and decrease the variability among the concentrations when performing statistical calculations; this approach also ensures that the calculation of the mean and upper confidence limit on the mean will be non-negative);

  - set the status to non-detect for these concentrations, but use the concentrations as reported in statistical calculations [this approach will not alter the mean concentration or the variability among the concentrations when performing calculations; however, the risk assessor should carefully review the statistics that are calculated to make sure they make sense (e.g., if a particular statistic such as the upper confidence limit on the mean is to be used as a representative concentration in risk calculations and this statistic is negative, the risk assessor should consider adjusting this statistic to the value of zero since negative concentrations may not make sense)]; and

  - use a surrogate concentration of the MDA (or some fraction of the MDA, such as 1/2 MDA) for all such data in the statistical calculations and set the detection status to non-detect for these data (this approach will generally increase the mean concentration and decrease the variability among the concentrations when performing statistical calculations; this approach also ensures that the calculation of the mean and upper confidence limit on the mean will be non-negative).

— Verify that identical records (i.e., specific samples entered into the data set more than once) are not present in the data set. When identical records are identified, verify that the original data set contained these repeat values and inform the data custodian that this situation exists so that the identical records can be eliminated from the data set.

— Verify that there are no missing data entries in the data set. For example, there could be a missing sample point or an entire group of sampling data that was missed during the data entry process. When appropriate, the risk assessor should reference a work plan or a sampling and analysis plan to verify that all data are included in the data set. The risk assessor should also verify that the data set does not contain any records with missing concentrations. If there are missing concentrations, an explanation for this must be provided and the data custodian should be consulted.

— Check the data set for typographical errors [e.g.,characters (letters) that may have been entered instead of numbers or vice versa] and make appropriate corrections as necessary [e.g., the

uppercase letter O entered instead of the number zero (0), or the lowercase letter l entered instead of the number one (1)].

— Verify that groundwater and surface water samples are identified as either filtered or unfiltered in the data set. It is inappropriate to combine filtered and unfiltered water concentrations when statistically evaluating the water data.

— Perform the five times and ten times rules when the data have not been 100% validated and the QC data [i.e., the blank(s)] have been supplied to the risk assessor. The five times rule and ten times rule may need to be performed on validated data if the data validation did not incorporate these rules.

— Evaluate duplicate (or replicate) samples. Four common methods for evaluating duplicate sample data are:

  – use the largest concentration of the duplicate (replicate) or original samples (this method will result in the calculation of the most conservative risk value);

  – use the average concentration of the duplicate (replicate) and original samples (this method will result in the calculation of a mid-range risk value);

  – use the concentrations from the duplicate (replicate) and the original samples in the calculation of the representative concentration (this method can bias the particular sampling location); and

  – use only the concentrations from the original samples in the calculation of the representative concentration (i.e., consider the duplicate/replicate data to be quality control-type data that are not used in the data evaluation for the risk assessment).

— Evaluate radiological data (if available) to ensure project team decisions pertaining to the data are met. Special consideration should be given to the evaluation of radiological data in the risk assessment. Without this consideration, radiological risks that are calculated may be grossly overestimated or of poor quality. Three specific situations that should be evaluated are:

  – Determine how risks are to be calculated for parent and short-lived daughter isotopes (this should be a project team decision). If the risk assessor plans to use the "+D" slope factors (which include contributions from the parent and short-lived daughter isotopes) then the data set being evaluated (i.e., the data set with concentrations) should be adjusted accordingly to avoid "double-counting" risks. This requires knowledge of decay chains and how "+D" slope factors are calculated (i.e., which short-lived daughters are included in the calculation of the "+D" slope factor for the parent isotope). For example, consider a data set that contains both ^{234}Th and ^{238}U data (^{234}Th is one of several short-lived daughter products of ^{238}U; for this example, assume that all other short-lived daughters of ^{238}U are not included on the data set). If the data set contains concentrations from both of these isotopes and the risk assessor plans to evaluate ^{238}U using the "+D" slope factors, then unless ^{234}Th is eliminated from the Chemicals of Potential Concern (COPCs) list, there is a chance of double-counting the risk associated with the ^{234}Th isotope [since its risk would be "counted" with the "+D" slope factor from ^{238}U (as applied to the ^{238}U concentration), as well as being "counted" with the slope factor for ^{234}Th (as applied to the ^{234}Th concentration)]. In this situation (when both ^{238}U and ^{234}Th data are present), the risk assessor should (1) eliminate all of the ^{234}Th data, evaluate the ^{238}U data (i.e., determine if ^{238}U is a COPC), and apply the "+D" slope factor on the ^{238}U data; or (2) use the "regular" (i.e., not the "+D") slope factor for ^{238}U and the "regular"

slope factor for ^{234}Th (^{234}Th does not have a "+D" slope factor), and evaluate the ^{238}U and ^{234}Th data independently of each other (applying the "regular" slope factors to the respective isotopic data). Note that there are many parent/daughter relationships that need to be examined by the risk assessor; the relationship between ^{238}U and ^{234}Th is just one of many possible relationships that fall into this category. The risk assessor is responsible for addressing all such relationships to ensure that risks from radionuclides are not "double-counted."

- Determine if the ratios of the radiological data are in the range of expectation. A simple plot of ratios of the reported concentrations from the two isotopes in question should suffice. As an example, if the concentrations of two particular isotopes are expected to be approximately the same, then the risk assessor can plot the values of the ratios (concentration of isotope-1/ concentration of isotope-2) against the sample order (from 1 to N, where N is the total number of sample results available). If the calculated ratios do not fall along the value of 1 (the expected ratio), the risk assessor should perform further investigation to determine the cause and make a decision about the data usability.

- Determine if the quality of the radiological data warrants using surrogate data, based on parent/daughter relationships. If radiological data are of questionable quality for a specific isotope for a known reason, the risk assessor should examine the relationship of this particular isotope in the radiological decay chain, and where possible, consider using surrogate concentrations for these questionable data. For example, consider a data set containing ^{226}Ra, ^{214}Pb, and ^{214}Bi concentrations (^{214}Pb and ^{214}Bi are two of several short-lived daughter products of ^{226}Ra; also suppose that no other short-lived daughter products of ^{226}Ra are found on the data set being evaluated). Suppose that for a known reason, the reported concentrations for ^{226}Ra are of poor quality (e.g., its concentrations are too large due to interferences from photopeaks of another isotope). Suppose also that the reported concentrations of ^{214}Pb and ^{214}Bi are of high quality (e.g., concentrations are in the "expected" range and based on the method of evaluation, there are no interferences from photopeaks of other isotopes). The risk assessor can use the fact that ^{226}Ra is a member of a radiological decay chain to infer its activity from the activity of its associated decay products (i.e., short-lived daughters). The radionuclide ^{226}Ra produces equal activities for its five daughter products after approximately 30 days (i.e., the activities are "in equilibrium"). In this case, since the activities of the daughter products (^{214}Pb and ^{214}Bi are the only two daughter products on the data set being evaluated) in this decay series should be equal to the parent (^{226}Ra), it is possible to infer/predict the activity of the parent when the activity of the daughter radionuclides is known. In the situation described above, ^{214}Pb and ^{214}Bi should be examined to demonstrate that they produce expected results. The risk assessor can examine the levels of reported concentrations, as well as plot ^{214}Pb concentrations against ^{214}Bi concentrations to ensure that the concentrations from these two isotopes mirror each other. Based on the scenario described, the risk assessor can use the average concentration of ^{214}Pb and ^{214}Bi to predict the concentration for ^{226}Ra and use this concentration as the surrogate concentration for ^{226}Ra.

— Identify outliers/hot spots. No standard formula or method for identifying outliers exists. Therefore, a method developed by Tukey (*Exploratory Data Analysis*, 1977) may be used for the identification of outliers. The upper and lower limits identified by this process are known as the outer fences. Concentrations beyond these outer fences are considered to be outliers. This method is a distribution-free method for identifying outliers:

- Determine 25th and 75th percentiles (P25 and P75).

  Upper limit = P75 + 3*(P75-P25)
  Lower limit = P25 - 3*(P75-P25)

– Evaluate data points versus upper limit and lower limit. Any concentrations that are smaller than the lower limit or larger than the upper limit are considered to be outliers. If outliers are identified, review the sample location, date, time, etc., to determine if patterns exist in the data that might explain why the outlier is different from other data. This may be an indication of a hot spot. Extreme caution should be used before eliminating data from the data set based on the outlier test. The risk assessor should not eliminate any outliers from the data set unless overwhelming evidence is found, and a concise reason for excluding data from the data set must be presented in the risk assessment.

B.4 PERFORM CALCULATIONS AND TESTS ON THE DATA

The risk assessor must calculate summary statistics for each analyte within each area of potential concern for each medium of potential concern in that area and then determine the frequency of detection for each analyte. The following two categories may emerge for frequency of detection: (1) all concentrations are nondetects (e.g., 0/24 detected); within this category of analytes, those analytes that have valid toxicity values will have their detection limits evaluated in the HHRA by comparing the largest reported detection limit versus the appropriately chosen risk-based PRG; and (2) at least one concentration for the analyte is detected (e.g., 1/24, 15/24, or 24/24 detected).

In determining the best-fit distribution for the concentrations of each analyte, the following factors must be considered:

- How will nondetects be used in the characterization of the concentrations? Many options are available, including:

  — assigning the reported detection limit as the concentration for the nondetect,

  — assigning one-half of the reported detection limit as the concentration for the nondetects,

  — assigning the nondetected concentration to be zero for the nondetects, and

  — evaluating the distribution of the detected values and statistically determining the distribution of the lower tail (i.e., the nondetected concentrations) for each analyte.

- How will the risk assessor determine the best-fit distribution of the data? The best-fit distribution should not be limited to the normal or lognormal distributions. If another distribution can be determined more appropriate, that distribution should be used to evaluate the analyte concentrations. Many possible approaches may be used to determine a best-fit distribution. One valid approach is to perform hypothesis testing, where the null hypothesis is that the concentrations come from a specific distribution (e.g., a normal distribution). There are many different statistical tests from which to choose. Some general information/suggestions about hypothesis testing follows.

  — To test the hypothesis that the data are normally distributed, the Shapiro-Wilk test (for small sample sizes) or the Kolmogorov test (for large sample sizes) can be used. The output includes the appropriate p-values; however, these two tests are valid only when treating all concentrations as detects. Comparing p-values from the results of several different null hypotheses may be used as a method for determining the data's appropriate distribution. For example, if the test for normality produces a p-value of 0.35 and the test for lognormality produces a p-value of 0.10, the risk assessor could then choose the normal distribution as the distribution to be used in the

remaining analyses (since it had a larger p-value than the lognormal p-value and since the p-value of 0.35 was acceptably large).

— Testing the logs of the concentration data for normality is equivalent to testing the untransformed concentration data for normality.

— In the event that the risk assessor cannot find a distribution that appropriately fits the data (e.g., if all p-values from the hypothesis testing are less than 0.001), then a nonparametric approach to the data evaluation is a legitimate option [e.g., the Product Limit Estimator approach (Schmoyer et al. 1996)].

- Summary statistics for each analyte should then be calculated. The statistics to be calculated include: (1) minimum and maximum detected concentrations, (2) minimum and maximum nondetected concentrations, (3) mean concentration, based on the appropriately chosen distribution, and (4) upper 95% confidence limit (UCL95) on the mean concentration based on the appropriately chosen distribution.

- The summary statistics should be presented in a table format and include :

  — analyte name,
  — frequency of detection,
  — distribution used,
  — range of detected concentrations,
  — range of nondetected concentrations,
  — mean concentration,
  — UCL95 on mean concentration, and
  — units of measure.

- Where appropriate, statistically compare the historical and current data for each analyte, testing for differences between mean concentrations and between the variances of the concentrations. The decision to compare these two sets of data should be a project team decision; appropriate statistical tests (consult a statistician when necessary) should aid in the decision to include/exclude historical data in the HHRA. The suggested level of confidence to be used in these statistical tests is a 95% confidence level. Factors that need to be weighed in choosing the appropriate statistical tests include the:

  — sampling design for each set of data,
  — quantity of data available for each set of data,
  — frequency of detection for each set of data, and
  — distribution (normal, lognormal, etc.) for each set of data.

- Where appropriate, statistically compare areas within the area of potential concern.

- The same logic applies here as presented previously, but with the purpose of determining whether to evaluate the area of potential concern as a whole (in terms of an HHRA) or to evaluate smaller areas within the larger area.

B.5 EVALUATE ANALYTES TO BE CONSIDERED AS QUANTITATIVE AND QUALITATIVE CHEMICALS OF POTENTIAL CONCERN

- Eliminate analytes with all nondetects from the COPCS list (with the exception of known site-related contaminants). The detection limits of all such analytes will be further evaluated in the HHRA by comparing the largest detection limit versus the appropriately chosen risk-based PRG.

- Eliminate analytes that are detected less than 5% (e.g., frequency of detection = 1/20) of the time at the same sampling location (EPA 1989).

- Evaluate tentatively identified compounds (TICs) per *Risk Assessment Guidance for Superfund, Part A* (RAGS) (EPA 1989a) for each area/medium combination and determine the number of TICs present and the number of analytes on the Target Analyte List (TAL) or Target Compound List (TCL). Next, report basic summary statistics for each TIC (e.g., number of results, minimum, maximum, and mean concentrations, etc.) and determine if TICs are to be evaluated further in the HHRA.

  — If only a few TICs are present compared to the TAL and TCL chemicals and no historical or other site information indicates that either a particular TIC may indeed be present at the site (e.g., because it may be a by-product of a chemical operation conducted when the site was active) or that the estimated concentration may be very high (i.e., the risk would be dominated by the TIC), then generally do not include the TICs in the HHRA.

  — When many TICS are present relative to the TAL and TCL compounds identified or if TIC concentrations appear high or site information indicates that TICs are indeed present, then further evaluation of TICs is necessary.

  — Consult with the project team about omitting TICs from the quantitative risk assessment and document reasons for excluding TICs from the HHRA.

- Compare sample data with background data. Eliminate analytes from the COPCs list if concentrations are not statistically different from background or if concentrations are significantly below background. Appendix C contains detailed guidelines on statistical approaches for background comparisons.

- Evaluate essential human nutrients per RAGS guidance (EPA 1989a, EPA 1995a). Essential human nutrients (e.g., iron, magnesium, calcium, potassium, chloride, phosphorus, iodine, and sodium),which are present at low concentrations and toxic only at very high doses, do not need to be evaluated in the quantitative HHRA. However, a quantitative comparison of essential human nutrients versus appropriate reference concentrations (i.e., compare against the Recommended Daily Allowances) should be made.

- Perform a screening using chemical-specific, risk-based PRGs (hereafter referred to as PRGs) to eliminate analytes that have valid toxicity values, but do not significantly contribute to total excess lifetime cancer risks (ELCRs) and hazard indexes (HIs), from the COPCs list for the quantitative risk assessment (EPA 1995a).

  — Perform this screen using the PRGs provided on the RAIS (LMER 1998). Compare analytes to PRGs for the exposure pathways being evaluated in the HHRA; the appropriate land use(s) and exposure pathways for screening are those deemed necessary to support remedial decisions.

Analytes for which the maximum detected concentrations are less than the PRGs (at ELCR ≤ 1E-06 and/or hazard quotient ≤ 0.1) for the appropriate scenario may be eliminated from the quantitative risk assessment. When both carcinogenic and noncarcinogenic PRGs are available for an analyte, only analytes whose maximum detected concentration is smaller than both PRGs may be eliminated from the COPCS list.

- Compare nondetected chemical quantitation limits to risk-based PRGs.

  — The reported detection limits for all nondetected chemicals (i.e., analytes that are not detected in any/all samples) should be compared to PRGs to ensure that the detection limits were appropriate (i.e. low enough). A table should be generated as a result of this comparison and the results should be discussed in the text of the HHRA, especially if the reported detection limit for a specific analyte exceeds the PRG.

- Identify quantitative and qualitative chemicals of potential concern.

  — Analytes not eliminated by the evaluations listed previously are considered to be COPCs. Those analytes that have valid toxicity (refer to the RAIS, LMER 1998) values will be further evaluated quantitatively in the HHRA, while those analytes that do not have valid toxicity values should be evaluated qualitatively in the HHRA.

APPENDIX C

BACKGROUND COMPARISON

This guidance directs the user through the process of performing background data versus sampling data comparisons for risk assessments performed under the auspices of the U.S. Department of Energy Oak Ridge Operations (DOE-ORO) sites. It provides a consistent and scientifically defensible approach for performing background comparisons by individuals or parties performing quantitative risk assessments. This guidance is consistent with the *Risk Assessment Guidance for Superfund: Volume I - Human Health Evaluation Manual, Part A (RAGS Part A)* (EPA 1989a).

The following information outlines the steps necessary to perform a background concentration comparison for risk assessments. The purpose of this comparison (i.e., the comparison of site data to background data) is to eliminate analytes from the chemicals of potential concern (COPCs) list that have concentrations less than background concentrations. These steps are outlined sequentially in relation to the background comparison process.

C.1 BACKGROUND DATA CHARACTERIZATION

- Evaluate detection limits prior to the calculation of any statistics for the background data.

- Characterize background concentrations for inorganic chemicals and naturally occurring radionuclides.

- Whenever any type of media of potential concern (e.g., soil, groundwater, surface water, etc.) is evaluated at one of the ORO sites (i.e., at Oak Ridge, Paducah, and Portsmouth), the risk assessor should use the appropriate medium-specific background data to meet the objectives of the risk assessment.

- Whenever the site soil data are evaluated for an Oak Ridge Reservation (ORR) site, the risk assessor should use the background soil data provided in the Background Soil Characterization Project (DOE 1993) for the background comparison/screening.

> **Note:** an extensive background characterization (for inorganic analytes) has been performed for the Oak Ridge Y-12 Plant (Y-12) groundwater (LMES 1996b); these background characterizations should be utilized as deemed appropriate.

C.2 GENERAL APPROACH FOR COMPARING BACKGROUND DATA

- Determine a background upper 95% tolerance limit (UTL95) concentration with 95% coverage for the distribution of the appropriate background data.

- Use the background UTL95 concentration as the "cutoff" for determining if site data are below background.

  — If any single *detected* concentration from the site data is above the background UTL95 concentration, then there is evidence that the site data's distribution is different from the background data's distribution; in this situation, one concludes that the site data are "above" background.

  — Site analytes that have <u>all</u> detected concentrations at or below the background UTL95 concentration can be eliminated from the chemicals of potential concern (COPCs) list, based on this background comparison.

- When calculating the background UTL95 concentration, the risk assessor must be aware of the sample size, sample distribution (e.g., normal or lognormal), and frequency of detection for each background analyte. When only a few background data points are available, the estimates of the mean concentration and the variance may be poor; therefore, caution should be used when calculating the background UTL95 concentration based on small sample sizes.

- An effort should be made to evaluate outliers in the background data set (i.e., data points that are extreme values and that do not appear to belong to the background distribution) and if justified, to eliminate the outlier(s) from the background distribution, prior to the calculation of the background UTL95 concentration.

C.3 CALCULATIONS WHEN BACKGROUND DATA ARE AVAILABLE FOR ANALYSIS

- Calculate the UTL95 concentration for each analyte in the background data based on the best-fit distribution and the frequency of detection. There are three categories of data, based on the frequency of detection:

  — background frequency of detection is $\geq$50%,
  — background frequency of detection is between 0% and 50%, and
  — background frequency of detection is 0% (all nondetects).

  When the background frequency of detection is $\geq$50%, calculate the background UTL95 concentration according to the best-fit distribution (normal or lognormal distribution) for each analyte by:

  — testing the hypothesis that the data are normally distributed (H_o: Normal), using a 95% level of confidence;

  — testing the hypothesis that the data are lognormally distributed (H_o: Lognormal), using a 95% level of confidence; and

  — choosing the best-fit distribution based on results from these two tests.

    – If H_o: Normal results in a p-value $\geq$ 0.05 or if H_o: Lognormal results in a p-value $\geq$ 0.05, select the best-fit distribution based on the largest p-value. Then calculate the background UTL95 concentration parametrically, using the appropriately chosen distribution (normal or lognormal).

    – If H_o: Normal can be rejected at the 95% level of confidence (i.e., $p_N<0.05$), and if H_o: Lognormal can be rejected at the 95% level of confidence (i.e., $p_L<0.05$), then calculate the background UTL95 concentration nonparametrically.

- Calculate the background UTL95 concentration.

  — Parametric calculation

$$a) \quad Normal: \; UTL = \overline{x} + k(s_x)$$

where:

$\overline{x}$ = arithmetic mean of the background data,
k = appropriate tolerance factor for one-sided tolerance intervals (based on sample size), and
s_x = standard deviation of the background concentrations.

$$b) \quad Lognormal: \; UTL = \exp\,[\overline{y} + k(s_y)]$$

where:

exp = e (2.718281828),
$\overline{y}$ = arithmetic mean of the logs of the background data,
k = appropriate tolerance factor for one-sided tolerance intervals (based on sample size), and
s_y = standard deviation of the logs of the background concentrations.

— Nonparametric calculation

For sample sizes ≤59, the nonparametric UTL95 concentration = maximum detected concentration (Walpole and Myers 1978). For sample sizes >59, randomly select a subsample of size 59; the maximum detected concentration among the 59 concentrations is the nonparametric UTL95 concentration.

- After calculating the background UTL95 concentration (for each analyte), compare this UTL95 concentration to the maximum detected background concentration; use the smaller of these two concentrations as the "cutoff" for determining if site data are above background.

— When the background frequency of detection is between 0% and 50%, there is very little confidence that the background distribution can be adequately characterized (since more than half of the data points are most likely reported as quantitation limits). In this situation, use the 99th percentile of the background data as the "cutoff" for determining if the site data are above background.

— When the background frequency of detection is 0% (i.e., all nondetects) it is not appropriate to compare site data against background data.

C.4 CALCULATIONS WHEN ONLY BACKGROUND DATA SUMMARY STATISTICS FOR ARE AVAILABLE

The general approach taken in this situation (i.e., when only data summary statistics are available for the background data) depends on which specific statistics are available to the risk assessor. Several situations and corresponding approaches are discussed in the following text. The particular approach that should be used can be determined by following the prioritized list:

- The background UTL95 concentration is given.

— For background data/analytes with a frequency of detection of ≥50%, the risk assessor should use the background UTL95 concentration as the "cutoff" for comparisons with site data.

— For background data/analytes detected at a frequency < 50%, the risk assessor should use the maximum detected background concentration as the "cutoff" (unless the background 99th percentile is provided, in which case it should be used as the "cutoff") for comparisons with site data.

— For background data/analytes with a frequency of detection of 0%, it is not appropriate to compare/screen site data against background data.

- The background mean concentration and standard deviation (or variance) are given.

  — If the background frequency of detection is ≥ 50%, the risk assessor should calculate the background UTL95 concentration from the background mean and standard deviation (provided that the sample size is also given) for comparisons with site data.

  — If the background frequency of detection is between 0% and 50%, the risk assessor should use the maximum detected background concentration as the "cutoff" (unless the 99th percentile is provided, in which case it would be used as the "cutoff") for comparisons with site data.

  — If the background frequency of detection is 0%, it is not appropriate to compare site data with background data.

- The background mean concentration is given, but no measure of variation (i.e., standard deviation or variance) is provided.

  — Use 2 times the background mean concentration (2 x [mean]) as the "cutoff" for comparing site data to background data (EPA 1995a).

  — For background analytes with all concentrations as nondetects, it is not appropriate to compare/screen site data against background data.

- No background mean concentration is given, but the background median concentration is provided.

  — Use 2 times the background median concentration (2 x [median]) as the "cutoff" for comparing site data to background data (EPA 1995a).

  — For background analytes with all concentrations as nondetects, it is not appropriate to compare/screen site data against background data.

C.5 HOW TO COMPARE (SCREEN) SITE DATA WITH BACKGROUND DATA

- Evaluate each analyte that has both background data and site data. Whenever any *detected* concentration from the site data (for a given analyte) is larger than the background "cutoff" concentration, there is evidence that the site data are above background and the analyte should remain on the COPCS list. In other words, if the maximum detected concentration from the site data (for a given analyte) is larger than the corresponding background “cutoff” concentration, that (site data) analyte is considered to be above background and should remain on the COPCS list.

- If site data (concentrations) are all nondetects (for a given analyte), the comparison with background is not necessary since these analytes have been (or will be) eliminated from the COPCS list based on detection status.

APPENDIX D

GUIDE FOR AIR DISPERSION MODELING FOR RISK ASSESSMENT

D.1 INTRODUCTION

The Oak Ridge Reservation (ORR), which consists of Oak Ridge National Laboratory (ORNL), Oak Ridge Y-12 Plant (Y-12 Plant), and the Oak Ridge K-25 Site (K-25 Site), was placed on the National Priorities List in 1989 and, as such, is required to comply with the requirements of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), commonly referred to as Superfund after the Superfund Amendments and Reauthorization Act of 1986 (SARA). In addition to the three installations, the lands used by Oak Ridge Associated Universities and waterways that have been contaminated by releases from the ORR are also included in the CERCLA designation.

The nature of the wastes treated, stored, or disposed of at the ORR sites is heterogeneous and often unknown. Under CERCLA, the United States Department of Energy (DOE), the Tennessee Department of Environment and Conservation (TDEC), and the United States Environmental Protection Agency (EPA) share a common goal to ensure that releases of hazardous substances, associated with past waste management and operational activities at the ORR, are adequately investigated and that appropriate remedial action is taken to protect human health and the environment (Miller 1995).

This report presents guidance for conducting air dispersion modeling analyses for CERCLA sites on the ORR. In many cases, the complex nature of atmospheric dispersion makes exposure via the air pathway more difficult to predict than exposure via other pathways. The air pathway is unique in that any on-site release of emissions can have an almost immediate impact on the air quality of the surrounding area. Furthermore, the impact locations can shift relatively quickly with changes in wind speed and wind direction.

Another complicating factor is the unavailability of methods for mitigating the consequences of a release after the contaminants enter the atmosphere. In contrast, exposures through other pathways (i.e., groundwater, surface water) often occur over extended time periods and can be minimized by limiting site access or prohibiting use of contaminated resources (e.g. drinking water).

Developing and implementing an air dispersion modeling program can be approached in a systematic manner but cannot be reduced to simple “cookbook” procedures. Professional judgement is needed as well as flexibility when selecting applicable models and appropriate input parameters for use on the ORR. Modelers benefit from having a technical background in source characterization, air monitoring, and risk assessment. In addition, modelers must perceive the strengths and limitations of a model before applying it to a specific situation. Model application should proceed only after the modeler understands the technical formulation, features, and assumptions incorporated into the model.

The primary objective of this report is to offer technical guidance for atmospheric dispersion modeling to contractors conducting baseline studies and FSs on the ORR CERCLA sites. Another objective of this report is to provide a summary of exposure scenarios, approaches for source-term characterization, and summary of air dispersion models useful for ORR baseline and FS risk assessments. In addition, this document identifies sources for site-specific data and references for additional information. The report uses many of the concepts identified in EPA Volume V, *Procedures for Air Dispersion Modeling at Superfund Sites* (EPA 1995). Subsequent sections of this white paper present exposure scenarios, typically considered in baseline studies and Feasibility Studies (FS); source characterization; and attributes of specific radionuclide and chemical contaminant air dispersion models are summarized. Finally, parameters typically used in air dispersion models are discussed. In addition, for certain parameters, ORR information resources are provided.

D.2 LAND USE—EXPOSURE SCENARIOS

EPA's Superfund program currently defines exposure scenarios within the context of four land use classifications: residential, commercial/industrial, agricultural, and recreational. EPA evaluates residential exposure scenarios when residential homes are located on or near a contaminated site or when future residential development is a reasonable expectation. Five pathways are routinely evaluated under the residential exposure scenario:

- direct external radiation from photon-emitting radionuclides in the soil,
- inhalation of resuspended contaminated dust,
- inhalation of radon and radon decay products (only when radium is present in soil),
- ingestion of contaminated drinking water, and
- ingestion of contaminated soil.

Two additional pathways (i.e., consumption of contaminated homegrown produce and consumption of contaminated fish) are also considered at some residential sites but only when site-specific circumstances warrant inclusion.

EPA evaluates occupational exposure scenarios whenever the land use is or may be commercial or industrial. These scenarios typically assess adult worker exposures by assuming an exposure occurs during an 8-hour work day, 5 days per week, 50 weeks per year for 25 years. Exposure pathways considered under this scenario are identical to those evaluated for the residential exposures, with the omission of pathways for consumption of fish and homegrown produce.

EPA evaluates agricultural scenarios whenever individuals live or work in contaminated areas zoned for farming activities such as growing crops or raising livestock. Under this scenario, EPA assumes that family members are exposed via the same five principal pathways evaluated for individuals under the residential setting, plus the mandatory inclusion of the plant pathway (i.e., consumption of home-grown produce). EPA also considers additional pathways for the ingestion of contaminated beef and dairy products, but only when such pathways are valid, considering the site conditions and lifestyles of the populations.

Under the recreational exposure scenario, EPA includes pathways for consumption of locally caught fish—both for subsistence and recreation—and for dermal exposures that might occur during swimming and wading. Fish ingestion pathways are evaluated only when there is access to a contaminated water body large enough to produce a consistent supply of edible-sized fish.

D.3 SOURCE TERM DERIVATION

Unlike other environmental pathways, the air pathway is characterized by short migration times, relatively large exposure areas, and the inability to mitigate the consequences of a release after the contaminants enter the atmosphere. Exposure times may range from only a few minutes to many years. The very nature of the air pathway is conducive to producing errors in the measurement or prediction of the fate of airborne contaminants over time and distance. Since these difficulties exist, a two-step approach is recommended. The first step is to use a screening-level approach for deriving a source emission rate. Initially, a mass loading factor (particulate) or default emission factors/rates can be used. If using these conservative factors results in a potential noncompliance or health hazard, the second step is to develop site-specific parameter values to derive source emission rates.

D.3.1 Source Definition

Each emission source and the constituents emitted by each source must be specifically identified. An important first step in defining a source term is to characterize each emission as a point, area, volume, or line source. It is also important to identify the locations of sources and the spatial extent of fugitive sources. General characteristics of several sources associated with baseline (pre-remediation), remediation, and post-remediation activities are shown in Table D.1. The source classification as well as the primary air emission mechanisms are summarized. Each source may have a fundamental release classification and, in some cases, multiple classifications.

Table D.1. General characteristics of sources associated with remedial technologies

Source	Source Classification	Release Classification	Air Emission Mechanisms Gas Phase	Air Emission Mechanisms Particulate Phase
Pre-remediation				
Landfills	Fugitive (area)	Gas release from solid Fugitive particulate	Volatilization	Wind erosion, mechanical disturbance
Lagoons	Fugitive (area)	Low volatility release from liquid	Volatilization	n/a
Contaminated Soil	Fugitive (area)	Gas release from solid Fugitive particulate	Volatilization	Wind erosion, mechanical disturbance
Containers	Fugitive area, volume	Gas release from solid Low volatility release from liquid High volatility release from liquid Gas release Fugitive particulate	Volatilization	Mechanical disturbance
Storage Tanks	Fugitive (area)	Gas release from solid Low volatility release from liquid High volatility release from liquid Gas release	Volatilization	n/a
Remediation				
Soil handling	Fugitive area, volume	Gas release from solid Fugitive particulate	Volatilization	Wind erosion, mechanical disturbance
Air Stripper	Point	Gas release	Volatilization	n/a
Incinerator/ Thermal desorption	Point	Gas release Fugitive particulate	Combustion	Combustion
In situ Venting	Point	Gas release	Volatilization	n/a

Table D.1. (Continued)

Source	Source Classification	Release Classification	Air Emission Mechanisms Gas Phase	Air Emission Mechanisms Particulate Phase
Solidification/ Stabilization	Fugitive area, volume	Gas release from solid Fugitive particulate	Volatilization	Wind erosion, mechanical disturbances
Post Remediation				
Landfills	Fugitive (area)	Gas release from solid Fugitive particulate	Volatilization	Wind erosion, mechanical disturbance
Soil Surfaces	Fugitive (area)	Gas release from solid Fugitive particulate	Volatilization	Wind erosion, mechanical disturbance

Most sources are ground level or near ground, nonbuoyant releases, except for small stacks where the plume is frequently influenced by downwash in the wake of nearby structures.
Source: EPA 1995

Many of the current refined dispersion models can accommodate a large number of sources. The manner in which a particular source is addressed depends on a number of factors. For example, a large area source such as a landfill may be subdivided into multiple, smaller area sources. This method allows for any spatial or temporal variability in emissions over the source as a whole. Furthermore, a remediation technology, such as excavation, can be subdivided into separate emission sources. For example, excavation of a pit would represent one emission source, the area over which the excavated materials are transported would be another emission source, and the short-term storage piles would be a third emission source.

D.3.1.1 Point source characterization

Point sources are characterized by the release of emissions from a well-defined localized source such as a stack or vent. Consequently, characterizing point sources for modeling is fairly straightforward. The basic model inputs for a point source are:

- stack height above ground level,
- inside diameter of stack,
- exit gas velocity or flow rate,
- exit gas temperature,
- building dimensions (e.g., building downwash), and
- emission rate.

The source and receptor locations must be defined. A receptor grid is often used by the models to establish receptor location. The influence of air pollution equipment (e.g., wet absorbers or scrubbers for incinerators, carbon absorption units for in situ venting, etc.) also needs to be considered. The presence of air pollution control equipment can alter the gas exit temperature and flow, both of which can effect plume buoyancy. The particulate size distribution may be altered as well due to the presence of air pollution control equipment (EPA

1995).

In the event that multiple point sources exist at a site, it may be possible to treat all of the emissions as if they were coming from a single representative stack at a central location. Merging stacks is appropriate under the following conditions (EPA 1995):

1. The individual point sources emit the same pollutants.

2. The individual point sources have similar stack parameters.

3. The individual point sources are located within 100 meters (m) of each other.

4. The maximum distance between any two stacks is small relative to the distance between any one of the stacks and the closest receptor.

D.3.1.2 Fugitive Source Characterization

Fugitive sources are generally divided into three categories for dispersion modeling: area, volume, or line sources. These fugitive sources involve the release of emissions from a defined surface or depth of space. The amount of emissions released from a fugitive source is directly related to the site environmental conditions (e.g., ambient temperature, wind speed above the surface, etc.) and the extent of mechanical disturbance (e.g., earthmoving agitation, transportation disturbance).

D.3.1.2.1 Area sources

Various types of toxic waste sources fall into the source category area: landfills, waste lagoons, evaporation and settling ponds, and areas of contaminated soils. For all of these sources, pollutants are emitted at or near ground level. The sizes of these sources can range from a few square meters in the case of settling ponds to a few square kilometers or larger in the case of contaminated soils. For dispersion modeling, the important parameters used to characterize area sources are :

- source location
- source geometry (dimensions)
- source height

Typically the emission rate or source strength for an area source is defined in amount of contaminant emitted per unit time per unit area [e.g., g/(s-m^2) or pCi/(s-m^2)]. In many models, area sources are defined by the location of the southwest corner of a square and a side length. An area source of irregular shape can be simulated by dividing the area source into multiple squares and/or rectangles that collectively approximate the geometry of the source. If the source is not at ground level, a source height may be entered. If the release height of the source is greater than approximately 10 m, it should be modeled as a volume source (EPA 1995). For additional information on modeling area sources, refer to *Review and Evaluation of Area Source Dispersion Algorithms for Emission Sources at Superfund Sites* (EPA 1989a).

D.3.1.2.2 Volume source characterization

A source is typically defined as a volume source when its emissions occur over a certain area and within

a certain depth of space. Two basic types of volume sources exist: ground level or elevated. An example of a ground level volume source is a surface rail line, and an example of an elevated volume source is an elevated conveyor. Fugitive exhaust from structures such as tanks or treatment facilities may be modeled as a volume source. However, fugitive exhaust can also be modeled as an area source. The parameters used to characterize volume sources for dispersion modeling include:

- source location,
- initial lateral dimensions, and
- vertical dimensions.

The length of a side of the volume source will need to be determined, as will the vertical height of the source. It is also important to note whether the source is on or adjacent to a structure or building.

D.3.1.2.3 Line sources

Line sources typically are used to represent roadways. Certain dispersion models differentiate line source from area or volume sources. In these cases, basic model inputs consist of:

- overall source length,
- source width, and
- source height.

Line sources may also be modeled as a series of area or volume sources.

D.3.2 Duration of Source Emissions (Continuous Versus Instantaneous)

Model selection for a particular emission scenario is based, along with other attributes, upon the geometry of the source and the duration of the emissions. Typically, the emissions from a source are categorized as being either instantaneous or continuous. Instantaneous emissions occur over a relatively short time span; whereas, continuous emissions are of a longer duration. Table D.2 summarizes the modeling emission duration categories associated with particulate, gas, and liquid emissions.

Table D.2 Summary of modeling categories for area and point sources

Initial Form of Release	Type of Release	Modeling Category
Particulate Matter	Stack	Continuous Point
	Fugitive Dust	Continuous Area
	Duct Failure	Instantaneous Volume
Gases	Flares	Continuous Point
	Stacks, relief valves, vents	Continuous Point
	Gas leaks: tanks, pipes, pumps, compressors	Continuous Point
	Multiple fugitive emissions	Continuous Area
	Land treatment emissions	Continuous Area
	Landfill emissions	Continuous Area
	Equipment openings	Instantaneous Volume
Liquids	Surface impoundments (quiescent)	Continuous Area
	Surface impoundments (aerated)	Continuous Area
	Continuous relief valve discharge	Continuous Point
	Instantaneous relief valve discharge	Instantaneous Point
	Liquid leaks: pipes	Continuous Area
	Liquid leaks: tanks	Continuous Area
	Liquid leaks: pipes (high volatility)	Continuous Point
	Liquid leaks: tanks (high volatility)	Continuous Point

Source: EPA 1988.

D.3.3 Methodology for Estimating Emissions

Two primary types of risk assessments that are typically conducted at ORR CERCLA sites are the baseline and FS assessments. The baseline risk assessment is conducted to assess risks from an undisturbed site; whereas, the FS assessment compares the risks generated by various site remedial alternatives. The following subsections summarize methods for estimating airborne emission rates from sources typically evaluated in baseline and FS risk assessments.

D.3.3.1 Baseline Risk Assessments—Emission Estimation

The use of formulations and models for estimating emission rates and ambient air concentrations does not

preclude the use of techniques for measuring emission rates or ambient air concentrations. Where site-specific conditions (e.g., a heterogeneous distribution of contaminants, a lack of reliable meteorological data, a heightened concern by community/states) do not lend themselves to these predictive techniques, more detailed techniques may be necessary.

The EPA has developed a guidance document (EPA 1992) to provide a series of sequential steps for conducting a baseline air pathway analysis. The EPA guidance document recommends the use of preferred EPA predictive models.

Typically, fugitive dust and gaseous emissions from undisturbed sites are evaluated in baseline risk assessments. Methods for estimating fugitive dust emissions include resuspension factors, mass loading factors, and emission rates/factors. For gaseous emissions, emission factors or emission rates are used.

D.3.3.1.1 Resuspension factors

Resuspension of contaminated soil has been recognized as a potential mode of human exposure for a number of years. However, methods for expressing the contaminant air concentrations resulting from resuspension have been quantitatively crude; in most cases, a resuspension factor has been used. There are generally three types of resuspension: (1) wind-driven resuspension, (2) mechanical resuspension, and (3) local resuspension. Both mechanical and local resuspension result from mechanical disturbance of soil; however, the dispersion patterns of the particulates differ. Mechanical resuspension factors are used for estimating contaminant air concentrations downwind of the source. Local resuspension pertains to resuspension in the immediate vicinity of the receptor before dispersion occurs (Healy 1980).

Studies of wind erosion of desert sands and agricultural soils have provided much of the information used to determine resuspension factors. Resuspension factors have, in many cases, not been used appropriately. Resuspension factors are not recommended for use in determining contaminant air concentrations because of the failure of the factors to account for many important variables. Conditions under which the factors are determined are not described in enough detail to allow extrapolation to areas different from those upon which the factors are based.

D.3.3.1.2 Mass loading factors

The mass loading concept is an attempt to bypass the details of the soil characteristics and resuspension process and relate directly measured contaminant concentrations in soil to the air concentration by use of the mass of the soil particulate. Using mass-loading factors is preferred to using resuspension factors. However, mass-loading factors must consider the distribution of contamination in soil. The air concentration of the contaminant is determined as the product of the contaminant concentration in the soil and the concentration of the soil particulate in the air. Therefore, measured dust loading factors for a particular region can be used to estimate contaminant air concentrations.

The mass loading factor of 100 $\mu g/m^3$ developed by Anspaugh for ambient air has no component for mechanical disturbance (Healy 1980). For cases with mechanical disturbance, a mass loading factor of 200 $\mu g/m^3$ is recommended for generic studies and is considered very conservative for estimating contaminant air concentration when compared to air sampling data (Healy 1980).

Mass loading factors are applicable for screening level assessments. For detailed analyses, emission rates

using measured data or site-specific parameters are preferred to using a mass loading factor.

D.3.3.1.3 Emission rates

Predictive modeling techniques involve calculating theoretical emission rates for both gaseous and particulate matter contaminants. Emission rate models predict emission rates as a function of contaminant concentration and contaminant physical and chemical properties within the surrounding media (e.g., soil, surface water, groundwater) and through measured or theoretically derived mass transfer coefficients. Many emission rate models have been evaluated against pilot-scale and field test results.

Many of these emission rate models require physical data (e.g., soil porosity, moisture content, etc.) about the surrounding media as well as physical and chemical properties of the contaminants (e.g., Henry's Law constants, diffusivity in air, etc.). Proper use of emission rate models requires that a thorough site characterization be conducted and that media-specific concentrations of all contaminants are adequately determined within the site volume in all three dimensions (i.e., all contaminant-specific "hot-spots" have been identified to a known depth). The emission rates calculated from these models must accurately represent the site or gross under/overprediction of the ambient air concentrations will result. Emission rate methods for use in baseline risk assessments are summarized in Appendix A.

D.3.3.2 Feasibility Study Assessments—Remediation Technology Emission Estimation

Contaminated environmental media (e.g., soil, groundwater, and surface water) can become disturbed by the implementation of technologies that may produce volatile organic compound (VOC) and particulate emissions. Additionally, the remedial technologies themselves (e.g., incinerators, air strippers, soil vapor extraction units) can emit VOCs and particulates by fugitive emissions or direct off-gassing. Contaminant emissions from disturbing environmental media or from operation of treatment technologies are released into the air where they become available for inhalation or ingestion. Implementation of remediation technologies can potentially increase baseline or undisturbed emissions and may impact the local air quality for both on-site workers and the surrounding population.

Many documents prepared by the EPA provide methods for assessing air impacts from various remediation technologies. However, cases do exist where the air quality impacts have not been fully characterized. Assessing the air impacts from various clean-up alternatives occurs prior to the actual clean-up process; therefore, FS studies must rely on estimated emissions and ambient air concentrations rather than on field measurements. The EPA Office of Air Quality Planning and Standards (OAQPS) has developed a "Technical Guidance Study Series" to provide assistance in estimating air impacts from a variety of remediation technologies. See Appendix B for an annotated list of these documents. By their very nature, these guidance documents contain procedures for estimating ambient air concentrations.

Remedial technologies can be divided into four major categories based on the type of contaminant emissions typically associated with the technologies: VOC point sources, VOC area sources, particulate point sources, and particulate area sources. Table D.3 shows a list of common remedial technologies and their associated categories. A variety of remedial technologies can be used to clean up CERCLA sites at DOE facilities. Not all types of remedial alternatives will be applicable to every site. In addition, not all remediation technologies will have an air pathway impact. The ambient air impacts of each applicable remedial alternative for a CERCLA site should be considered in the evaluation performed during the FS.

Technology-specific emission rates can be used by atmospheric dispersion models for estimating contaminant air concentrations. When site-specific emission rates are not known, EPA default emission rates may be used. However, actual measured emission rates, if available, are generally preferable to generic emission rates for use in the models. Default emission rates and methods for estimating emission rates for typical remedial technologies are summarized in Appendix A. In addition, Appendix A provides a detailed summary of default emission rates associated with typical remedial technologies.

Table D.3. Remedial technologies and associated source type categories

Source Type Category	Associated Remedial Technologies
VOC point sources	Air strippers
	Soil vapor extraction units
	Thermal desorption units
	Thermal destruction units (incinerators)
Particulate point sources	Thermal destruction units (incinerators)
	Thermal desorption units
VOC area sources	Excavation
	Dredging
	Solidification/stabilization
	In situ vitrification
Particulate area sources	Excavation
	Materials handling
	Solidification/stabilization
	Dry surface impoundments

D.4. MODEL SELECTION

Making the appropriate model selection depends, among other considerations, upon the following key factors (EPA 1995):

- site-specific goals,
- dispersion modeling objectives, and
- legal and liability aspects of the remediation project.
- pragmatic aspects of the program, including:

  — quality and availability of input data, including the ability of the emission models to adequately simulate emission rates and their variability;

— applicability of existing dispersion models to site-specific characteristics including source types;

— ability of existing dispersion models to reasonably simulate transport and dispersion of air pollutants released from the site, given the chemical, radiological, and physical processes involved; and

— ability to accomplish the dispersion modeling objectives with modest uncertainties.

According to EPA (1995), determination of the proper model to use for air dispersion modeling can be divided into a general two-step procedure for assessing air quality impacts. This two-step procedure involves an initial screening-level analysis to obtain conservative estimates of air quality based on limited data, followed by a refined analysis as necessary to provide more realistic estimates of air quality.

In general, screening level studies are performed to define the nature and extent of a problem and are considered conservative, particularly for long-term predictions. Screening studies are often used to eliminate the need for more detailed modeling of a particular situation. Refined studies are performed to provide more detailed treatment of atmospheric processes and source-receptor relationships and, at least theoretically, a more accurate estimate of source impact.

Screening evaluation activities are most likely to occur during the site investigation (SI), early remedial investigation (RI), or operation and maintenance (O&M) steps of the Superfund process. Refined evaluations are most likely to occur during the RI, FS, and O&M steps. At the ORR, determination of whether a screening-level or refined model should be selected for a risk assessment should be made with input from the Risk Assessment Manager.

EPA has approved numerous models for use in regulatory applications. Nonregulatory models also may be used if they can be shown to be more suitable for a given scenario. In cases where a modeler has developed a code for a certain application, EPA has developed a guidance document that identifies the steps necessary to have the code approved (EPA 1984, Cox 1988). It is recommended that EPA approved codes be used to conduct atmospheric dispersion modeling for risk assessments conducted on the ORR.

Since dispersion models are periodically revised, the model user should verify that the most updated version of the code is being executed. For models issued by the OAQPS, the model user should check the Support Center for Regulatory Air Models (SCRAM) Bulletin Board System (BBS).

For this report, the most generally applicable and commonly used air dispersion models (i.e., codes) are mentioned. The following subsections contain brief descriptions of codes used for estimating contaminant air concentrations and radionuclide doses from radionuclides at specific receptor locations. The applicability and limitations of the codes and the resulting output data are described. It is the responsibility of the modeler to ensure that the most appropriate techniques are selected.

D.4.1 Radionuclide Contaminant Codes

Table D.4 summarizes screening and refined dispersion models used for evaluating the impacts of airborne radionuclide releases. Paragraphs briefly describing each model are also included.

Table D.4. Summary of atmospheric transport codes for radionuclides applicable for baseline and FS assessments

	RASCAL	MILDOS-AREA	HOTSPOT	CAP88-PC	GENII	GENII-S	MEPAS	RESRAD	COMPLY	PRESTO*	PATHRAE-EPA*	COMMENTS
APPLICATION:												
Type												
Screening	X		X					X	X			
Detailed		X		X	X	X	X			X	X	
Multi-media					X	X	X	X		X	X	
Uncertainty analysis						X	X	X				
"User-friendly"	X	X	?	X	X	X	X	X	X			
SOURCE INFORMATION:												[a]Only U-238 chain as particulates; Rn-222 & daughters as gases. [b]Also resuspension estimated using resuspension factor. [c]MEPAS incorporates emission rate calculation method. [d]For off-site estimates, input is calculated using resuspension factors and burn factors) for dust suspension, and incineration or trench fires, respectively.
Activity released												
Input amount airborne	X	X	X[b]	X	X	X	X		X	X		
Estimate -												
Mass loading factors								X		X	X[d]	
Emission rate calc.							X[c]				X[d]	
Input concentrations	X				X	X						
Input chi/Q												
Particulate release	X	X[a]	X	X	X	X	X	X	X	X	X	
Gaseous release	X	X[a]	X	X	X	X	X	X	X	X	X	
Radioactive decay	X	X	X	X	X	X	X	X		X	X	
SOURCE TYPE:												[a]Virtual point-source estimation. [b]MEPAS specifies source type. But not for air pathway. [c]Handles area source by using "virtual point source using width of facility. [d]Soil or water contamination only.
Point	X	X	X	X	X	X	X		X	X	X	
Area		X	X[a]	X			X	X			X[d]	
Volume							X					
Line							X[b]					
Other												
Multiple sources		X		X			X[c]		X			

Table D.4. (continued)

	RASCAL	MILDOS-AREA	HOTSPOT	CAP88-PC	GENII	GENII-S	MEPAS	RESRAD	COMPLY	PRESTO*	PATHRAE-EPA*	COMMENTS
SOURCE RECEPTOR:												[a]Cumbersome hookup to external code. [b]COMPLY intended for use at ≤3 km. [c]Depends on which PRESTO code used. [d]Inhalation on-site to workers during operation from trench fire, incineration., &/or dust suspension; off- site pop. during operation and after closure.
Near-field	X	X	X	X	X	X			X[b]	X[c]	X[d]	
Far-field	X	X	X	X	X	X	X	X[a]		X[c]	X[d]	
On-site	X		X		X	X		X	X	X[c]	X[d]	
RELEASE DURATION:												
Continuous (chronic)		X	?	X	X	X	X	X	X	X	X	
Acute (unintentional)	X		X		X	X						
Intermittent (time variant)		X										
ATMOSPHERIC TRANSPORT:												[a]Box model assumes complete mixing. [b]COMPLY has different levels of assessment. [c]Input total deposition rate as input.
Gaussian plume	X	X	X	X	X	X	X	X	X	X	X	
Puff model	X											
Box model							X[a]	X[a]				
Wet deposition	X			X			X		X[b]	X[c]	X[c]	
Dry deposition	X	X	X	X			X		X[b]	X[c]	X[c]	
Gravitational settling		X		X					X[b]	X[c]	X[c]	
Building wake effects (downwash)	X				X	X	X		X	X		

Table D.4. (continued)

	RASCAL	MILDOS-AREA	HOTSPOT	CAP88-PC	GENII	GENII-S	MEPAS	RESRAD	COMPLY	PRESTO*	PATHRAE-EPA*	COMMENTS
METEOROLOGY:												[a]Input as assumed single wind speed, direction, and stability category. [b]Various sets of met. data from airports and government sites to choose in code if site-specific not available. In current version, another program needed to manipulate site-specific file. [c]Atmospheric transport handled only when coupled with another code. [d]Only input one average wind speed and stability in direction of receptor.
Site-specific input	X[a]	X		X	X	X	X	[c]	X			
Generic (or default)			X	X[b]			X	[c]		X[d]	X[d]	
TERRAIN:												
Simple	X	X	X	X	X	X	X		X	X	X	
Complex							X					
RELEASE HEIGHT:												[a]Only input effective release height. [b]No stack releases; only contaminated soil or water.
Ground-level	X	X	X	X	X	X	X	X	X	X[a]	X	
Elevated	X	X	X	X	X	X	X		X	X[a]	X	
Buoyant			X	X	X	X	X		X	X[a]	X	
PATHWAY OPTIONS:												[a]Inhalation dose from tritiated water vapor includes skin absorption. [b]Inhalation of radon in house built on-site; suspended dust on-site and off-site; of airborne particulates off-site. [c]External gamma from waste on- site. [d]Not from air transport; from use of contaminated water for direct consumption or irrigation only.
Inhalation	X	X	X[a]	X	X	X	X	X	X	X	X[b]	
Immersion in contaminated air	X	X	X	X	X	X	X		X			
Ground surface exposure	X	X		X	X	X	X	X	X		X[c]	
Dermal contact							X					
Ingestion: Terrestrial food chain		X		X	X	X	X	X	X		X[d]	
Ingestion: Animal product food chain		X		X	X	X	X	X	X		X[d]	
Ingestion: Inadvertent soil					X	X	X	X	X			
Ingestion: Surface water					X	X	X	X	?		X[d]	
Ingestion: Ground water					X	X	X	X	?			
Aquatic food					X	X		X	?		X[d]	

Table D.4. (continued)

	RASCAL	MILDOS-AREA	HOTSPOT	CAP88-PC	GENII	GENII-S	MEPAS	RESRAD	COMPLY	PRESTO*	PATHRAE-EPA*	COMMENTS
OUTPUT:												[a]Output only as input measured air concentrations. [b]Output results for various times.
Doses:												
Individual effective dose equivalent:	X	X[b]	X	X	X	X	X	X	X	X	X[b]	
Individual maximum				X	X	X	X	X				
Individual average (mean)	X		X	X	X	X				X		
Organ		X		X	X	X						
Collective					X	X					X[b]	
Cumulative				X	X	X	X	X		X	X[b]	
Per radionuclide	X			X	X	X	X	X		X	X[b]	
Per pathway												
Air Concentration:												
Total		X	X									
Per radionuclide	X[a]	X		X								
Chi/Q Receptor Location:												
Total					X	X					X	
Per radionuclide				X								

D.4.1.1 Screening-level codes

D.4.1.1.1 COMPLY

The purpose of the COMPLY program is to provide a means for facility operators to demonstrate compliance with the 40 CFR 61, Subpart I (10 mrem/yr). COMPLY is also a useful tool for evaluating the possible effects new radionuclide emission sources would have on the compliance status of a facility. For example, planned point sources can be evaluated before construction, and appropriate emission controls can be incorporated into the design of an emissions unit. However, the program cannot be used to demonstrate compliance with emission standards like 40 CFR 61, Subpart H, except under certain circumstances. EPA Rule 40 CFR 61.93(a) indicates that DOE facilities, where the maximally exposed individual lives within 3 km of all sources of emissions in the facility, may use EPA's COMPLY model and associated procedures for determining dose for purposes of compliance.

The COMPLY program estimates an annual effective dose equivalent (EDE) to a receptor from continuous releases of radionuclides from point sources. COMPLY can be used to evaluate multiple point sources simultaneously. In addition, the program can be run on an IBM or IBM-compatible personal computer (PC).

The COMPLY program has four screening levels of increasing complexity so that, with minimum effort, the analyst can choose the appropriate level and demonstrate compliance. If compliance cannot be demonstrated at Level 1, the analyst can proceed to a higher level that uses fewer assumptions, requires additional data input, and therefore results in a less conservative dose estimate. This process can be followed through all four levels. Level 1 consists of a set of radionuclide possession limits and concentration tables. If the facility meets these criteria, then the facility can demonstrate compliance with 40 CFR 61, Subpart I, without any further analysis. Levels 2, 3, and 4 estimate doses and are useful for evaluating planned radionuclide emission sources. Based on the screening level selected, input data may include a wind rose, stack parameters, distances to farms that may provide food for the receptor, and radionuclide release rates. The user's guide for the COMPLY code provides clear instructions for executing the program (EPA 1989a).

D.4.1.1.2 RESRAD

DOE Order 5400.5, Chapter IV, provides guidelines for deriving soil limits for residual radioactive materials. The RESRAD code was developed for estimating doses, predicting risks, and deriving site-specific guidelines for allowable residual concentrations of radionuclides in soil. These guidelines are primarily applicable for the time the property is released for unrestricted use.

RESRAD is a pathway analysis code that calculates radiation doses to a hypothetical individual residing on a contaminated site. RESRAD Version 5.6 allows the user to define up to nine pathways and three exposure routes as summarized Table D.4. Several scenarios, including residential, industrial, and recreational, can be modeled by adding or suppressing pathways and then entering appropriate values for the occupancy and consumption rates. A user's manual entitled "Manual for Implementing Residual Radioactive Material Guidelines Using RESRAD, Version 5.6" is currently available from the Radiation Shielding Information Center (RSIC). There have been many versions and revisions of the code; therefore, it is important to obtain the latest version of the code [for assistance, contact Dr. C. Yu at Argonne National Laboratory, phone: (708) 252-3144].

RESRAD is designed for use on an IBM or IBM-compatible PC and includes internal help files for information on input and output data. The code consists of three modules:

- RESPC, an interactive module for data entry and display;
- RESMAIN, the main calculational and report-generating module; and
- RESPLOT, an interactive graphics module that displays the latest RESMAIN results.

RESRAD Version 5.6 has several improvements compared to earlier versions (e.g., Version 3.12): These improvements include:

- calculation of potential health effects (excess risk cancer incidence),
- interactive graphics,
- performance of sensitivity analysis on most RESRAD parameters,
- multiple pathways, and
- optional user selection of all dose conversion and related factors including cancer incidence slope factors.

The particular strengths of RESRAD as compared to the other codes (i.e., MMSOILS and MEPAS) are:

- inclusion of database with the model;
- ability to perform an uncertainty analysis;
- availability of model parameter estimation guidelines;
- differential transport of ingrowth daughter in groundwater; and
- special models for tritium, carbon-14, and radon.

The RESRAD model has the following limitations relative to the other two models:

- limited source type availability,
- no multiple source/receptor capability,
- no internal capability for offsite assessments, and
- cumbersome off-site air transport pathway procedures.

For the on-site dust inhalation pathway, RESRAD has a default value for mass loading of dust in air (2.0E-4 g/m^3). RESRAD is the only model that considers the size of the contaminated area when adjusting doses; however, the area factor for inhalation calculated by RESRAD is close to one (0.97) for an area of 10,000 m^2 and does not greatly affect the results (Faillace 1993). In addition, occupancy and shielding factors are also used to estimate doses from the inhalation pathway. The default value of 0.45 is derived by assuming 25% outdoor occupancy, 50% indoor occupancy with 40% of dust originating from contaminated soil, and 25% off-site occupancy.

The current version of the RESRAD code is designed for estimating on-site individual doses. Off-site doses can be estimated by using a computer code such as CAP-88 or for uranium series nuclides, MILDOS-Area (ANL 1993). In the ANL report (1993), a simplified approach is suggested when external off-site dose codes are unavailable [refer to Appendix K in the ANL report (1993) for an explanation of this approach]. It is

strongly recommended that external codes developed for estimating off-site doses be obtained and used particularly when refined modeling is required.

RESRAD does not have the capability of estimating airborne fugitive dust emissions; these can be calculated by methods previously described or a generic dust release rate can be calculated using the mass loading factor (ANL 1993). These release rates can be input into the external codes to calculate doses to off-site individuals or the collective population.

D.4.1.1.3 RASCAL

The Radiological Assessment System for Consequence AnaLysis (RASCAL) code was designed to provide a rough dose estimate for comparison with EPA's Protective Action Guidelines (PAGs) and threshold for acute health effects. RASCAL is an emergency response screening model that can be used to conduct dose and consequence projections. The model can be run on any DOS system and is menu-driven with output displayed in text or maps.

RASCAL estimates dose and consequence from an accidental ground-level or elevated release (as a single point source) of radionuclides to the atmosphere. RASCAL also has the capability of computing both acute and chronic dose and dose equivalents from known environmental activity in the air and on the ground surface. Decay and daughter ingrowth are included. In RASCAL 2.1, the source term can be input directly (either as isotopic release rates or concentrations) or calculated. Three methods are available for estimating source term, but they are considered very crude estimates since detailed plant conditions cannot be known during an actual accident. The maximum allowable release duration is 24 hours. Decay and daughter ingrowth are assumed to begin at shut down time and end when the environmental release begins. The models used within RASCAL for atmospheric transport include either a straight-line Gaussian plume or a Gaussian-puff trajectory (for >2 miles). Four sets of meteorological data, consisting of date, time, surface wind speed and direction, stability class, mixing layer, and precipitation rate, can be entered with each set. The first set of data corresponds to the start of the release with the following sets in chronological order.

RASCAL was designed for distances of <100 km (near- and far-field). The code treats the atmosphere as having two layers. The lower layer lies between the ground and the height of the mixing layer where the wind speed is increasing with height. The upper layer is above the mixing layer, and the wind speed is assumed to be constant. The stability class chosen for these layers determines the diffusion within the layer while the wind direction is assumed to be the same for both. Both wet and dry deposition for particulates are considered in RASCAL. Noble gases are not affected by these processes. RASCAL also includes cloud-shine doses using a finite-puff model.

RASCAL output includes total acute bone dose and acute lung dose for early health effects evaluation. Total effective dose equivalent (50-year dose commitment) and thyroid and cloud-shine dose are used to compare with EPA PAGs. These comparisons provide a “snapshot” of integrated dose to a person (adult) standing outside (i.e., unshielded). Inhalation and cloud-shine doses are included for duration of exposure to the plume. For additional information refer to RASCAL, Version 1.3 (NUREG/CR-5247) and 2.1 (DRAFT; NUREG/CR-5247, Vol. 1, Rev. 2).

D.4.1.1.4 HOTSPOT

The HOTSPOT health physics codes were created to provide health physics personnel with a fast, field-

portable calculational tool for evaluating accidents involving radioactive materials. Hotspot codes are a first-order approximation of radiation effects associated with the atmospheric release of radioactive materials.

Four general programs—Plume, Explosion, Fire, and Resuspension—calculate a downwind assessment following the release of radioactive material resulting from a continuous or puff release, explosive release, fuel fire, or area contamination event.

The code uses a Gaussian plume dispersion model to determine the ground-level air concentrations at various locations downwind (near- and far-field). HOTSPOT considers point sources and area sources (estimated as virtual point source). Ground-level, elevated, and buoyant releases are covered in the codes.

Particulate and gaseous releases can be modeled with HOTSPOT. Deposition, resuspension of particulate, and radioactive decay are included in HOTSPOT's atmospheric transport model. Exposure pathways evaluated in HOTSPOT are inhalation of contaminated air and external exposure due to air immersion. Exposure to surface water and groundwater are not included.

The dosimetric methods of ICRP Publication 30 are used in HOTSPOT. The 50-year committed effective dose equivalents from resuspended material are calculated per one-hour residence time. The codes include a fairly extensive list of radionuclides. [For additional information, contact S. Homann (510) 423-4962 and refer to *HOTSPOT, Health Physics Codes for the PC*, UCRL-MA-106315, Lawrence Livermore National Laboratory, March 1994.]

D.4.1.2 Refined models

D.4.1.2.1 CAP-88

The CAP88/CAP88-PC computer code estimates the dispersion and transfer of radionuclides in the terrestrial environment. CAP88-PC is a PC version of the mainframe version CAP-88. Unless otherwise noted, CAP-88 will be used as a generic reference denoting both versions. The computer code implements a Gaussian plume atmospheric dispersion algorithm, and the terrestrial pathway equations are similar to those cited in the U.S. Nuclear Regulatory Commission (NRC) Guide 1.109 (NRC 1977).

The CAP-88 model is applicable for evaluating individual and population doses from chronic releases. The model includes algorithms for evaluating plume rise through buoyancy; depletion of plumes through radioactive decay, precipitation scavenging, gravitational settling, and dry deposition; and wet and dry deposition on ground surfaces. The CAP-88 computer code can estimate doses from area (i.e., circular only) or point sources. Table D.4 summarizes selected attributes of the CAP-88.

The CAP-88 model is composed of three modules: (1) PREPAR, which is a preprocessor for AIRDOS-EPA data; (2) AIRDOS-EPA, which calculates atmospheric dispersion, estimates radionuclide concentrations in the environmental media, and predicts radionuclide intakes; and (3) DARTAB, which calculates doses and risks based on the concentrations and intakes calculated in AIRDOS-EPA.

CAP-88 calculates the EDE and cancer risks to individuals and populations through exposure pathways that include inhalation of contaminated air, ingestion of contaminated food, and external exposure to contaminated ground surfaces. The dose and risks can be reported by nuclide, organ, or exposure pathway (EPA 1990).

The primary difference between the CAP88-PC and CAP-88 is that the user is able to access and change more default input data in CAP-88, which allows the user to conduct more site-specific assessments. If the default data are satisfactory for the user's purpose, CAP88-PC is easier to use and has the advantage of running on a PC. The user can create and edit files in the program shell which simplifies the model's use. The required input data are brief and relatively easy to obtain. The CAP88-PC user's manual is brief and easy to follow but is not as comprehensive as the CAP-88 user manual. Therefore, for more information on the theory of the models, consult the CAP-88 user's manual.

CAP-88 and CAP88-PC generally produce more conservative results than its counterpart GENII except for ground level releases (Maheras 1994, Fields 1994). Specifically, CAP-88 produces lower EDEs than GENII for ground level releases since CAP-88 accounts for plume depletion by dry and wet deposition, which may be an important factor to consider when choosing a model (Maheras 1994).

CAP-88 and CAP88-PC are approved by the EPA for demonstrating compliance with 40 CFR Part 61, Subpart H, “National Emission Standards of Radionuclides Other Than Radon From Department of Energy Facilities” (DOE 1994). CAP88-PC and CAP-88 are available from the RSIC [P.O. Box 2008, ORNL, Oak Ridge, Tennessee, 37831, phone: (615) 574-6176].

D.4.1.2.2 GENII

GENII is a radiological assessment computer code system that estimates individual and collective doses to humans from the environmental transport of radionuclides in the atmosphere, surface water, and other environmental media and includes biotic transport and manual redistribution to the surface from buried waste (Maheras 1995). Table D.4 summarizes the attributes of GENII and the GENII-S codes.

GENII consists of seven linked computer codes and their associated data library. The codes are: APPRENTICE, ENVIN, ENV, DOSE, EXTDF, INTDF, and DITTY. APPRENTICE is a preprocessor with a series of interactive menus that allow quick and easy entry of input data. Default parameters are provided for most data. APPRENTICE checks user input values to ensure that the data are reasonable. APPRENTICE prepares a text input file for calculating doses and a batch file that controls file handling for ENVIN, ENV, and DOSE. ENVIN, ENV, and DOSE are the programs executed to calculate the dose. These programs are the most commonly used programs in GENII.

EXTDF, INTDF, and DITTY are computer codes used for special calculations. EXTDF performs external dose and shielding evaluations for finite source geometries. INTDF calculates internal dose factors using ICRP-26/30 methods and can calculate internal dose factors for commitment periods greater than 50 years. DITTY calculates long term doses (i.e. 10,000 years) from waste disposal activities. These three programs are used less frequently and are generally less user friendly.

The atmospheric transport pathway in GENII is applicable for both chronic and acute releases, far-field and near-field scenarios, and ground level and elevated releases. GENII's atmospheric transport model is based on the Gaussian plume algorithm. Various equations may be used, depending on the release duration (i.e., 30 minutes to 4 hours or longer), for assessing an acute atmospheric release. Determination of which equation(s) should be used is based on an evaluation of the physical situation being modeled, source characteristics, and the meteorological situation (Napier 1988). GENII implements an acute version of a Gaussian plume atmospheric dispersion model and allows the user to choose the probability level associated with the

atmospheric dispersion during an acute release (Moore 1994). For acute releases, the models have been modified to account for acute deposition, contaminant movement through the food chain, and consideration of the four seasons' variations (Napier 1988).

GENII is a multimedia model that integrates a number of environmental pathways in one system. GENII uses equations and formulation found in other models. For example, for the chronic crop ingestion pathway, GENII uses equations similar to those found in Regulatory Guide 1.109 (NRC 1977). In other cases, GENII uses equations from other sources (e.g., for the terrestrial food pathway GENII uses the PATHWAY formulation). It is also unique, as compared to codes with similar applications, in that the user can bypass the environmental transport portion of the code and input either measured or estimated (using other codes) radionuclide concentrations in select media or food products. [GENII is distributed by RSIC and to obtain code specific information, contact B. Napier, Pacific Northwest Laboratories, Hanford, Washington, phone: (509) 375-3896.]

D.4.1.2.3 GENII-S

GENII-S is GENII with a built-in statistical analysis package that can produce statistical results as well as deterministic results. However, GENII-S cannot account for atmospheric dispersion uncertainty and radioactive decay during plume transport when used in the statistical mode. When used in the deterministic mode, GENII and GENII-S yield the same results (Maheras 1994).

One advantage of GENII-S over GENII is that the user can easily edit the input file. GENII-S allows the user to enter either a fixed value or a range of values for the input data. The user can specify fixed, normal, lognormal, triangular, uniform, or nonuniform distributions. The user can also obtain graphical results, statistical results, and other output data. In addition, the user can create cumulative distribution plots, complementary cumulative distribution plots, histograms, scatter plots, and X-Y plots. The statistical results produce maximum, mean, and minimum values of interest; the standard deviation; raw and rank correlation coefficients; and results from linear least squares fit. The user can choose a wide choice for output data. For example, the user can obtain statistical results of the EDE, the dose to the organ from the pathway or radionuclide, and/or a combination of these. [GENII-S was produced at Sandia National Laboratory (SNL). Dr. C. D. Leigh can provide information on how to obtain the model and can be contacted at Sandia National Laboratories, Albuquerque, New Mexico 87185, phone: (505) 844-1888.]

D.4.1.2.4 MEPAS

The Multimedia Environmental Pollutant Assessment System (MEPAS) is a physics-based risk computation code that integrates source-term, transport, and exposure models. It can be used for both radioactive and chemical contaminants. Currently, MEPAS is the only code with this capability.

MEPAS is applicable for use in both screening and assessment applications for baseline studies and FSs. It is designed for site-specific assessments and uses relatively standard transport and exposure computation approaches. However, a unique feature of MEPAS is that these approaches are integrated into a single system. It can be implemented on a PC and is considered to be user-friendly.

The basic characteristics of MEPAS are summarized on Table D.4. The MEPAS code comprises nine main components:

1. source term
2. overland pathway
3. groundwater (vadose and saturated zones)
4. surface-water pathway
5. atmospheric pathway
6. exposure routes
7. hazard assessment
8. contaminant transport/exposure
9. Chemical database

The first eight components are described by a set of standard algorithms that are contained in their own module. The transport pathway models are systematically integrated with the exposure assessment component that considers the type, time, and duration of exposure and location and size of the population exposed. The atmospheric pathway in MEPAS combines:

- release mechanisms and characteristics,
- dilution and transport,
- washout by cloud droplets and precipitation, and
- deposition on the underlying surface cover.

MEPAS can consider volatilization, suspension, plume rise, and complex terrain components. In addition, MEPAS allows back-calculation of emission rates from environmental monitoring data. Wind and mechanical suspension emission are based on a report by Cowherd (1985), while 5 types of volatilization emissions are based on reports by Thibodeaux (1989) and EPA (1988).

Transport and dispersion are computed in terms of a sector-averaged Gaussian dispersion model, which provides sector averaged contaminant concentrations for a downwind distance and height in a plume from a continuous source release. Deposition is computed as the sum of outputs from empirical wet and dry deposition algorithms.

Some of the strengths of MEPAS include:

- inclusion of a database with the model,
- multiple receptor capacities,
- ability to provide acute air dispersion information,
- special models for tritium and carbon-14,
- ability to perform an uncertainty analysis,
- availability of model parameter estimation guidelines, and
- ability to estimate population risks.

Some of the limitations of the MEPAS model are:

- a two-step process implements the MEPAS multimedia source-term module that partitions to multiple environments (however, the separate air and water source-term module used in other comparison cases are fully linked);

- no multiple source capability for the air pathway; and

- no methods for handling on-site assessments [concentrations at 100 m must be used for on-site evaluations; no model for on-site air dispersion estimates, e.g., box model (or indoor)].

This code is currently undergoing a benchmark study which is comparing the technical formulations and performance characteristics of MEPAS, RESRAD, and MMSOILS. It also has been compared to other codes, such as GENII. The MEPAS code is still in the early development stage; however, it is a multimedia code that can be used for both chemical and radiological contaminants and is applicable for assessing remediation alternatives at DOE facilities. [This code and associated users manual can be obtained from Pacific Northwest Laboratories, J. Buck, phone: (509) 376-5442.]

D.4.1.2.5 PRESTO/PATHRAE

The PRESTO family of codes was written to assist EPA in generating a standard for the land disposal of low-level radioactive waste which would support the NRC and DOE in developing a national waste management system. The PRESTO family of codes consists of:

- PRESTO-EPA-POP — Estimates cumulative population health effects to local and regional basin populations from land disposal of low-level waste by shallow methods; long-term analyses are modeled (generally 10,000 years)
- PRESTO-EPA-DEEP — Estimates cumulative population health effects of local and regional basin populations from land disposal of low-level waste by deep methods
- PRESTO-EPA-CPG — Estimates maximum annual whole-body dose to a critical population group from land disposal of low-level waste by shallow or deep methods; dose in maximum year is determined
- PRESTO-EPA-BRC — Estimates cumulative population health effects to local and regional basin populations from less restrictive disposal of "below regulatory concern" wastes by sanitary landfill and incineration methods
- PATHRAE-EPA — Estimates annual whole-body doses to a critical population group from less restrictive disposal of "below regulatory concern" wastes by sanitary landfill and incineration methods

Considering the source variability associated with remediation operations at DOE sites, one or more of these codes could potentially be of use. The following sections discuss the PRESTO-EPA-POP, PRESTO-EPA-CPG, and PATHRAE-EPA codes. In addition, a user-friendly PC Windows version of PRESTO is currently being developed.

PRESTO-EPA-POP. The PRESTO-EPA-POP code was the first code developed and served as the basis for the other codes. These codes are used to compare the potential health impacts of a broad number of low-level waste disposal alternatives. DWNWND is incorporated into the PRESTO family of codes for atmospheric dispersion. DWNWND is an interactive implementation of the Gaussian plume atmospheric dispersion model. Any one of eight different sets of empirically determined dispersion parameters can be selected to simulate different release heights and meteorological and terrain conditions. The choice allowance is what makes this code unique. The dispersion parameters sets available in DWNWND are Pasquill-Gifford, Briggs-Smith,

Briggs, Klug, Brookhaven, St. Louis, and Julich (for 50-m and 100-m release heights). Computed values can be corrected for plume depletion from deposition and gravitational settling.

PRESTO-EPA-CPG. The PRESTO-EPA-CPG code is designed to estimate radiation doses to individuals and critical population groups for a 1000 year period from disposal of low-level waste. On-site doses from farming and intrusion and off-site doses from exposure to contaminated air, surface water, and groundwater are estimated. The following on-site and off-site exposure pathways are considered:

1. inhalation of contaminated dust suspended in the air;

2. external dose from radionuclides in soil, water, and air; and

3. ingestion of contaminated plants, meat, milk, and water.

The atmospheric transport portion of the PRESTO code is handled internally by a version of the DWNWND code. The dose factors used by PRESTO are relatively old but can be modified by the user. The code output options include reporting doses by radionuclide, pathway, and organ but only for the time at which the maximum occurs. Daughter ingrowth and subsequent transport are not considered. A mass loading factor is used for generating a dust suspension source term.

PATHRAE-EPA. This particular member of the PRESTO family is expanded from the -CPG and -BRC codes by emphasizing two areas: (1) the addition of specific radionuclide exposure pathways regarding on-site workers during disposal operations and to off-site individuals after closure and (2) simplification of submodels to reduce computing time to run on a personal computer. PATHRAE-EPA is a multiple transport pathway annual dose assessment code. It allows for analytical solutions of transport equations. Both annual radiation doses and health effects can be projected for any time period during or following the end of low-level waste disposal operations.

Exposure pathways include contaminated groundwater transport to rivers or wells, surface water contamination by erosion, contamination of soil and water due to disposal facility overflow, atmospheric transport of airborne nuclides and inhalation by humans. Inhalation doses can be estimated for workers engaged in operations and for an off-site population during operation and after site closure. Annual doses can be estimated due to external exposure, inhalation, or ingestion of contaminated materials on or below the ground surface.

The atmospheric transport pathway has the option of estimating doses at off-site locations due to dust resuspension, waste incineration, or a trench fire. For doses from dust resuspension, a resuspension rate and deposition velocity are used. Burn rates and fractions are used when incineration or trench fires are considered.

PATHRAE-EPA can locate the position of the maximum dose for each individual nuclide as well as the time at which the maximum dose occurs. It also has the option of adjusting the nuclide inventory for decay during operation and for times beyond facility closure. The radionuclide inventory and cumulative risk and doses for the entire facility for each time considered is output along with the maximum annual dose, health risk, year of maximum health impact, and the dominant nuclide for each exposure pathway.

D.4.1.2.6 MILDOS-AREA

MILDOS was designed to compute environmental radiation doses from uranium recovery operations. It was originally developed for the NRC. The code uses a straight line crosswind-integrated Gaussian plume dispersion model to determine the incremental normalized ground-level air concentrations due to each source and radionuclide as a function of the meteorology. MILDOS considers both point sources and area sources.

The original MILDOS used a virtual-point method to approximate an area source. MILDOS-AREA, written for use on a PC and updated to include larger area sources and more recent dosimetry calculations, uses a finite-element integration scheme with the advantage of permitting large area sources to be partitioned into triangles, rectangles, or elements of other selected shapes. Irregularly shaped boundaries can be more accurately described with a minimum number of mesh points. The atmospheric concentration of particulates or gases from an area source can be determined by integrating a point-source dispersion concentration over an entire area.

Particulate daughters of ^{222}Rn are assumed to be not depleted due to deposition and not resuspended. Release of particulate is limited to ^{238}U, ^{230}Th, ^{226}Ra, and ^{210}Pb (and their daughters in secular equilibrium). Radon-222 and daughters are the only radionuclides included as gaseous releases. Deposition, radioactive decay, daughter ingrowth, and environmental weathering are all included in MILDOS. MILDOS allows the user to vary the source term with respect to time by adjusting the emission rates, including shutting them off completely. This could reflect changes in processes over time.

Exposure pathways considered in MILDOS are inhalation of contaminated air; ingestion of contaminated vegetables, meat, and milk; and external exposure due to air immersion and contaminated ground surfaces. Individual (including total commitments for all radionuclides in the code) and population doses (regional, extra-regional, total, and cumulative) are based on ICRP 30 dose conversion factors and are estimated for each of these pathways. Exposure to surface water and groundwater are not included.

MILDOS-AREA is the updated version of MILDOS and is designed to run on a PC. However, it is not considered to be “user-friendly” since it is not menu-driven.

For additional information, consult the following documents:

MILDOS - A Computer Program for Calculating Environmental Radiation Doses from Uranium Recovery Operations, NUREG/CR-2011, April, 1981.

MILDOS-AREA: An Enhanced Version of MILDOS for Large Area Sources ANL/ES-161, 1989.

D.4.2 Chemical Codes

Several atmospheric dispersion models are currently available for estimating chemical contaminant air concentrations from point and area sources. Table D.5 summarizes the attributes of a number of screening level and refined air dispersion models used to estimate chemical contaminant air concentrations. The remainder of this section provides a brief description of each model provided. All of the codes, with the exception of MEPAS and the box model, are EPA-approved and are available from the EPA Bulletin Board. [Contact D. Atkinson, EPA (919) 541-0518, for information on how to access the SCRAM bulletin board.]

Table D.5. Atmospheric transport codes summary for chemical contaminants applicable to baseline studies and FSs (OFCM 1993)

Attributes	CDM	CRSTR	FDM	ISC	CTDM+	MPTER	RAM	RTDM	SLAB	Valley	TSCREEN	PAL	MEPAS	COMMENTS
APPLICATION TYPE														
Screening										x	x	x		SLAB/TSCREEN: accidental spill
Detailed	x	x	x	x	x	x	x	x	x				x	ISC/RAM/RTDM/Valley/TSCREEN/MEPAS: application to elevated stack releases, (e.g., power plants)
Multi-media													x	
Uncertainty analysis													x	
Computer Type														ISC/TSCREEN/MEPAS: can be adapted to wide range of applications
PC	x	x	x	x	x	x	x	x	x	x	x	x	x	
Mainframe	x	x	x	x		x	x	x		x				TSCREEN: customized chemical database
Processing Mode														
Interactive		x	x								x	x	x	
Batch	x			x	x	x	x	x	x	x				
SOURCE INFORMATION														[1]Slab: Aerosol (two-phase release)
Particulate release		x	x	x		x	x				x	x	x	
Gaseous release	x	x		x	x	x	x	x	x[1]		x	x	x	
SOURCE TYPE														[1]MEPAS specifies source type but not for air pathway.
Point	x	x	x	x	x	x	x	x	x	x	x	x	x[1]	
Area	x		x	x			x		x	x	x	x	x	
Line	x		x	x								x	x	
Release Height														
Ground level	x	x	x	x	x	x	x	x		x	x	x	x	
Elevated	x	x	x	x	x	x	x	x		x	x	x	x	
Multiple sources	x		x	x		x	x			x	x		x	

Table D.5. (continued)

Attributes	CDM	CRSTR	FDM	ISC	CTDM+	MPTER	RAM	RTDM	SLAB	Valley	TSCREEN	PAL	MEPAS	COMMENTS
SOURCE RECEPTOR														
Far Field(< 100 km)	x	x	x	x	x	x	x	x	x	x	x		x	
Near-field				x							x	x	x	
On-site				x								x	x	
RELEASE DURATION:														
Continuous (chronic)														
Instantaneous	x	x	x	x	x	x	x	x	x	x	x	x	x	
Intermittent (time variant)				x					x		x			
ATMOSPHERIC TRANSPORT (Gaussian):														[1] Modification of MPTER (e.g., MPTDS) that explicitly accounts for gravitational settling and/or depositional loss of pollutant ISC3: incorporates Complex 1, requires terrain contour input if terrain is above stack height
Continuous plume	x	x		x	x	x	x	x		x	x	x	x	
Puff model											x			
Box model												x		
K-diffusion			x						x					
Plume Density: Light	x	x		x	x	x	x	x		x	x		x	
Plume Density: Neutral	x	x		x	x	x	x	x	x	x	x		x	
Plume Density: Heavy									x					
Wet deposition				x									x	
Dry deposition			x	x		x[1]					x		x	
Gravitational settling						x[1]						x		
Chemical Reaction	x													
Chemical TD-decay	x													
Surface Roughness			x		x	x			x					
Building wake effects (downwash)				x							x			
Terrain														
Simple (Flat)	x	x	x	x		x	x	x	x	x	x	x	x	
Complex				x	x			x		x				

Table D.5. (continued)

Attributes	CDM	CRSTR	FDM	ISC	CTDM+	MPTER	RAM	RTDM	SLAB	Valley	TSCREEN	PAL	MEPAS	COMMENTS
METEOROLOGY INPUT:														CRSTER/FDM/ISC/MPTER/RTDM: hourly wind data preprocessed with RAMMET CTDM+ surface and profile data processed with METPRO TSCREEN: met data input appropriate for screen, Puff, or RVD models.
Temperature		x	x	x	x	x	x	x	x		x	x	x	
Mixing depth	x	x	x	x	x	x	x	x			x	x	x	
Sky and solar conditions		x	x		x	x	x					x		
Point winds	x	x	x	x	x	x	x	x	x		x	x		
Wind profile/rose	x			x		x	x	x			x		x	
Vertical temperature profile				x	x	x	x	x			x			
Wind from multiple points					x									
PATHWAY OPTIONS:														MEPAS can be used to assess exposure routes, see radionuclide summary table for further information
Inhalation													x	
Immersion in contaminated air													x	
Ground surface exposure													x	
Dermal contact													x	
Ingestion													x	
OUTPUT:														[1]FDM: Deposition [2]Slab: Cloud temperature, density, height, width and entrainment velocities [3]TSCREEN: Plot of concentration vs distance [4]MEPAS: Hazard Quotients and Risks
Air Concentration:	x	x	x	x	x		x		x	x	x	x	x	
Other:			x[1]	x[1]					x[2]		x[3]		x[4]	

CDM: Climatological Dispersion Model, EPA
CRSTER: EPA
CTDM Complex Terrain Dispersion Model, EPA
FDM: Fugitive Dust Model, EPA
ISC: Industrial Source Complex, EPA
MPTER: Multiple Point Source Algorithm, EPA
RAM - EPA
RTDM: Rough Terrain Dispersion Model, EPA
SLAB: LLNL/USAF
Valley: EPA
TSCREEN: EPA
PAL: Point, Area, and Line, EPA
MEPAS: Multiple Environmental Pathway Assessment System, PNL/DOE

D.4.2.1 Screening codes

D.4.2.1.1 TSCREEN

TSCREEN, a model for screening toxic air pollutant concentrations, is a computer program that implements the procedures written in *A Workbook Of Screening Techniques For Assessing Impacts of Toxic Air Pollutants* (EPA 1988a). To correctly analyze toxic emissions and their subsequent dispersion from one of many different types of possible releases from Superfund sites, the TSCREEN should be used in conjunction with the accompanying workbook.

TSCREEN is an umbrella model composed of three different models: RVD (Relief Valve Discharge), Puff, and SCREEN. The RVD model is a screening technique applicable to denser-than-air gaseous releases. The Puff model is used for short-duration events or instantaneous passively dispersing puffs (e.g., emissions due to duct failure). SCREEN is primarily used for point sources with continuous emissions. It can be used to estimate contaminant air concentrations from gaseous, liquid, or particulate matter releases from stacks, vents, and fugitive or windblown dust emissions. Building downwash effects can be considered in the cavity recirculation zone for near wake and wake regions. SCREEN is limited in that it is a screening level model, and its input does not allow wind rose data.

Using TSCREEN, a particular release scenario is selected via input parameters, and TSCREEN automatically selects and executes the appropriate dispersion model to simulate that scenario. The model to be used and the worst case meteorological conditions are automatically selected based on criteria given in the workbook.

Although TSCREEN can be used as an area source model using a virtual point source procedure, EPA's Point, Area, and Line-Source Model (PAL) is more accepted for estimating contaminant air concentrations associated with area sources.

D.4.2.1.2 PAL

The PAL model is an atmospheric dispersion model used for estimating contaminant air concentrations. PAL can manage six different source types: point, area, horizontal line, special line, curved path, and special curved path. The foundation of the PAL model is the steady-state Gaussian plume point source equation that characterizes the dispersion and transmission of point source emissions. This equation uses the crosswind and upwind source-receptor distances, the effective emission height, source strength, and wind speed to produce air concentration evaluations. The Gaussian plume equation is used in a modified form for computations involving square or rectangular area sources. It is assumed that dispersion from area elements produces a Gaussian pattern distribution in the vertical and horizontal directions.

PAL initially divides the area source into nine crosswind line source segments. The first estimate of the contaminant air concentration from the area source is generated by performing an integration over the lines, which considers the contaminant concentration contribution from each line and the distance between lines. A second air concentration calculation is made by considering 10 lines lying midway between the 9 line segments, as well as the original 9 lines themselves, to determine a second concentration estimate. If the ratio of the two concentration estimates falls within a user-defined accuracy limit, the integrations stop; otherwise, the iteration continues (EPA 1989).

Only portions of the source area that are upwind of the receptor are accounted for in the integrations. If all corners of the area are in an upwind location, the PAL model performs an integration that proceeds from the site corner of minimum distance from the receptor to maximum distance from the receptor (EPA 1987). No computations are executed for sources that are entirely downwind from the receptor. A benefit of this model is that edge effects from the area source are taken into consideration.

The PAL model code has advantages over the box model in that it allows the user to input more detailed meteorological data, as well as precise worker configurations and specific properties of the contaminant such as the pollutant settling and deposition velocities. The exact position and height of the receptor point must be specified, which is advantageous for computing air concentrations at "on source" receptor points. For small area sources, the predicted air concentration is very sensitive to receptor height since the vertical dispersion is much less for these areas.

The Pasquill-Gifford rural dispersion coefficients can be employed by PAL to simulate a rural environmental setting. Gravitational settling of gaseous and particulate contaminants may also be accounted for in the PAL model. The PAL code can be used for estimating concentrations of nonreactive pollutants at 99 receptors for an averaging time of 1 to 24 hours.

The PAL algorithms have been evaluated for the use of area sources at Superfund sites (EPA 1989). Tests of mathematical and physical principles indicated that the PAL model produces physically reasonable results for all tests. These tests include stability comparisons, center versus edge, subdivisions, source orientation, and source height (EPA 1989). However, PAL model predictions are sensitive to source height.

D.4.2.1.3 SLAB

The SLAB model has been developed to simulate the atmospheric dispersion of denser-than-air releases over flat terrain. The model treats continuous, finite duration, and instantaneous releases from four types of sources: an evaporating pool, an elevated horizontal jet, a stack or vertical jet, and an instantaneous volume source. While the model is designed to treat denser-than-air releases, it will also simulate cloud dispersion of neutrally-buoyant releases. Consequently, a typical SLAB simulation covers both near-field dense gas phase and the far-field passive gas phase.

D.4.2.1.4 VALLEY

The Valley model is an analytical technique whose primary use is for estimating the upper limits of 24-hour average pollutant concentrations due to isolated sources in rural, complex terrain. Options are provided that allow multiple sources, flat terrain, urban areas, and long-term averages to be considered. The basic treatment of dispersion by the Valley model is quite similar to that of the Air Quality Display Model (AQDM) and the Implementation Planning Program (IPP). However, Valley includes modifications to the techniques used in these models, including (1) a representation of the effect of terrain on ground-level concentrations, (2) plume rise equations from Briggs, (3) a different treatment of pollutant reflection from inversions aloft, (4) a rural-area option, (5) a short-term option, and (6) printouts of the spatial distribution of concentrations on equal-area maps.

D.4.2.1.5 Box model

The semi-empirical Box model is the most elementary model in use for determining the atmospheric

dispersion of contaminants from an area source. It assumes that emissions from the source are uniform across the contaminated area. The area emission rate, or source strength, is the mass of contaminant emitted from the source per unit area per unit time. The dimensions of the contaminated area are designated as the box width and box length. The box length, box width, and mixing height define a volume into which all of the pollutants are evenly mixed. Instantaneous full mixing of the pollutants within the volume is assumed. The estimated contaminant air concentration represents an average throughout the volume; therefore, it is independent of position. A receptor inhaling contaminated air is assumed to be located inside the box, but the exact receptor height and position cannot be delineated. Convergent or divergent winds are not accounted for in this model. Therefore, the vertical motion of air has not been incorporated into the algorithm (EPRI 1979). Some box models allow the wind speed to change as a function of height above the ground; however, the wind speed can also be chosen to be constant within the layer between the ground surface and the mixing height (Ragland 1973). An advantage of the box model is that the equation for computing air concentrations is uncomplicated and does not require the use of a complex computer code.

D.4.2.2 Refined chemical codes

D.4.2.2.1 CDM

CDM-2.0 (Climatological Dispersion Model - Version 2.0) determines long-term (seasonal or annual) quasi-stable pollutant concentrations in rural or urban settings using average emission rates from point and area sources and a joint frequency distribution of wind direction, wind speed, and stability. The Gaussian plume algorithm forms the basis for the calculations. Contributions are calculated assuming the narrow plume hypothesis and involve an upwind integration over the area sources. Computations can be made for up to 200 point sources and 2500 area sources at an unlimited number of receptor locations. The number of point and area sources can be modified within the code. CDM-2.0 is an enhanced version of CDM and includes the following options:

- 16 or 36 wind-direction sectors,
- initial plume dispersion,
- buoyancy-induced dispersion,
- stack-tip downwash, and
- gradual (transitional) plume rise.

The user has a choice of seven dispersion parameter schemes. Optional output includes point and area concentration roses and histograms of pollutant concentration by stability class.

D.4.2.2.2 CRSTER

This algorithm estimates ground-level concentrations resulting from up to 19 colocated elevated stack emissions for an entire year and prints out the highest and second-highest 1-hour, 3-hour, and 24-hour concentrations as well as the annual mean concentration at a set of 180 receptor locations (5 distances by 36 azimuths). The algorithm is based on a modified form of the steady-state Gaussian plume equation that uses either Pasquill-Gifford or Briggs' urban dispersion parameters. It includes adjustments for plume rise and limited mixing terrain adjustments as long as the surrounding terrain is physically lower than the lowest stack height input. Pollutant concentrations for each averaging time are computed for discrete, non-overlapping time periods (no running averages are computed) using measured hourly values of wind speed and direction and estimated hourly values of atmospheric stability and mixing height.

D.4.2.2.3 CTDMPLUS

The Complex Terrain Dispersion Model (CTDM) is a point-source, steady state model for complex terrain applications. The model is unique in the way it simulates the flow and plume distortion near fully defined, three-dimensional terrain. Emphasis is given to windward side impacts. The algorithms for stable and neutral conditions are based on the concept of a dividing streamline. The algorithms for plumes released into convective layers are based on recent understanding of the convective boundary layer obtained through field, numerical, and fluid modeling studies (OFCM 1993).

D.4.2.2.4 FDM

The Fugitive Dust Model (FDM) is a computerized air quality model specifically designed for computing concentration and deposition impacts from fugitive dust sources. The sources may be point, line, or area sources. The model has not been designed to compute the impacts of buoyant point sources; therefore, it contains no plume-rise algorithm. The model is generally based on the well-known Gaussian plume formulation for computing concentrations, but the model has been specifically adapted to incorporate an improved gradient-transfer deposition algorithm. Emissions for each source are apportioned by the user into a series of particle size classes. A gravitational settling velocity and a deposition velocity are calculated by FDM for each class. Concentration and deposition are computed at all user-selectable receptor locations.

D.4.2.2.5 ISC

There is a short-term (ISCST) and a long-term (ISCLT) version of the Industrial Source Complex (ISC) code. These models contain a steady state Gaussian plume model which can be used to assess pollutant concentrations from a wide variety of sources associated with an industrial source complex. Both ISCST and ISCLT can account for the following conditions:

- settling and dry deposition of particulates,
  - downwash,
- area, line, and volume sources,
- plume rise as a function of downwind distance,
- separation of point sources, and
- limited terrain adjustment.

ISCST can estimate an average concentration or total deposition calculated in 1-, 2-, 3-, 4-, 6-, 8-, 12- and/or 24-hour time periods. An “n”-day average concentration (or total deposition) or an average concentration (or total deposition) over the total number of hours may also be computed. ISCLT is designed to calculate the average seasonal and/or annual ground level or flagpole concentration or total deposition from multiple continuous point, volume, and/or area sources. Provisions are made for special X, Y receptor points that may correspond to sampler sites, points of maxima, or special points of interest. Sources can be positioned anywhere relative to the grid system.

The complex terrain feature of COMPLEX1 has been included in the latest version of ISC (ISC3). COMPLEX1 is a screening algorithm for calculation of concentrations at receptors above stack height. In addition, improvements in the algorithms for area sources, deposition, pit retention, and wet deposition have been made in ISC3. This code is highly recommended by the EPA for air dispersion modeling (Tuoma 1995).

D.4.2.2.6 MPTER

MPTER is a multiple point source Gaussian model with optional terrain adjustment. MPTER estimates concentrations on an hourly basis for relatively inert pollutants (i.e., SO_2 and TSP). MPTER uses Pasquill-Gifford or Briggs' urban dispersion parameters and Briggs' plume rise methods to calculate the spreading and the rise of plumes. The model is most applicable for source-receptor distances less than 10 kilometers and for locations with level or gently rolling terrain. Terrain adjustments are restricted to receptors whose elevation is no higher than the lowest stack top. In addition to terrain adjustments, options are also available for wind profile exponents, buoyancy induced dispersion, gradual plume rise, stack downwash, and plume half-life.

D.4.2.2.7 MPTDS

MPTDS is a modification of MPTER that explicitly accounts for gravitational settling or deposition loss of a pollutant. Surface deposition fluxes can be printed under an optional output feature. MPTDS is a multiple point source code with an optional terrain adjustment feature. The code is primarily based upon MPTER which has Gaussian modeling assumptions. Execution is limited to a maximum of 250 point sources and 180 receptors. Hourly meteorological data are required. In addition the period of simulation can vary from 1 hour to 1 year.

D.4.2.2.8 RAM

RAM is a gaussian-plume multiple-source air quality algorithm. This short-term Gaussian steady-state algorithm estimates concentrations of stable pollutants from urban point and area sources. Hourly meteorological data are used, and hourly concentrations and averages over a number of hours can be estimated. Briggs' plume rise equation is used, and Pasquill-Gifford dispersion equations with dispersion parameters considered to be valid for urban areas are also used. Concentrations from area sources are determined by assuming that sources directly upwind are representative of area source emissions affecting the receptor (i.e., virtual point source). Special features include determination of receptor locations downwind of a significant source and determination of locations of uniformly spaced receptors to ensure good area coverage with a minimum number of receptors.

D.4.2.2.9 RTDM

The Rough Terrain Diffusion Model (RTDM) is a sequential Gaussian plume model designed to estimate ground-level concentrations in rough (or flat) terrain in the vicinity of one or more co-located point sources. It is designed for applications involving chemically stable atmospheric pollutants and is best suited for evaluation of buoyant plume behavior within about 15 km from the source(s). RTDM has special algorithms to deal with plume behavior in complex terrain.

D.4.3 Chemical/Radionuclide Codes

The only air transport code that can assess both radionuclide and chemical contaminants is MEPAS (see Sect. D.4.1.2.4). However, application of chemical codes to radionuclide contaminants are used as screening tools for estimating radionuclide concentrations at specific locations. Of course, these codes do not take into account radioactive decay and the ingrowth of progeny but can be used to assess a source type that can be better modeled with a particular chemical code.

D.5. PARAMETERS

The major input data components for air dispersion modeling analyses are (1) source characterization, (2) meteorological data, (3) receptor location, (4) rural/urban classifications, and (5) averaging time considerations. The dispersion models used to model airborne release of chemicals do not consider doses or risks, they typically furnish time-averaged air concentrations over a user-defined receptor grid. However, many of the dispersion models used to model airborne releases of radionuclides *do* consider individual and population doses and, in some cases, the associated risks. Therefore, codes applicable to radionuclide contaminants include exposure pathway parameters.

The input data can be grouped into three major categories: source-specific, site-specific, and study/task-specific. Table D.6 summarizes the type of data that typically falls into each of these categories and the resources for this information. See Sect. D.3 for a detailed discussion on source characterization. This section will discuss receptor locations, averaging time considerations, urban/rural classifications, and exposure pathway parameters.

Table D.6. Parameter and resource summary for air dispersion modeling

Parameters	Information Category	Resources
Source Characterization Source Term Release Duration Source Physical Parameters Number and Location	Source specific	Project and Facility Managers
Meteorological Data Ambient Temperature Rainfall Solar Radiation Atmospheric Pressure Wind speed and direction Stability Classes Joint Frequency Distribution	Site specific	Ron Sharp, CP&ED/OECD, ORNL [das@ORNL.gov] (has access to K-25 data and historical data from all 3 sites) Jim Grimes/Iris Shelton, Y-12 [GrimesJG@y12.gov] [SheltonID@y12.gov] Ed Bailiff/Ed Hatmaker, K-25 Kevin Birdwell, NOAA, ATDD [Birdwell@ATDD.NOAA.gov] (official NWS Data - daily precipitation and temperature, (daily-since 1940's; hourly data-last ten years) Since 1994: barometric pressure, humidity data, solar radiation, wetness FTP Server: Wind.ATDD.NOAA.gov Data/ORMET directory

Parameters	Information Category	Resources
Receptor Information Individual locations Population data	Site specific	Project Manager Sherri Cotter, OECD, ORNL [SHC@ORNL.gov] Richard Durfee, CP&ED, ORNL [DurfeeRC@ORNL.gov]
Exposure Pathway Information	Site/Program specific	Wilson McGinn, Risk Assessment Program [JSS@ORNL.gov] Frank O'Donnell, OECD, ORNL [FOD@ORNL.gov]

D.5.1 Meteorological Considerations

Meteorological conditions govern the transport and dispersion of contaminants and, in the case of some fugitive sources (i.e., lagoons or landfills), can affect the amount of the contaminant that becomes airborne. It is important to use meteorological data that are representative of the site area and vicinity. The following section provides basic information on the regional and local climatology. In subsequent sections, on-site meteorological data resources and guidance on worst-case impact determination are provided.

The EPA recommends that a minimum of either 1 year of on-site data or 5 years of off-site (e.g., National Weather Service) data are required to run refined dispersion models (EPA 1995). If long-term risk is an issue, it is desirable to have 5 or more years of on-site meteorological data to support long-term exposure assessments for refined air pathway assessments (EPA 1995).

D.5.1.1 Regional and local climatology

Local terrain in the vicinity of the ORR is mostly ridges and valleys, with ridge elevations generally between about 275 and 365 m (900 and 1200 ft) and with valley floors extending to the Clinch River. Orientation of the ridges and valleys is generally southwest-northeast, and the near-surface winds generally follow the orientation of the local topography. Elevation also influences temperature and precipitation patterns over the region, with cooler temperatures and greater precipitation generally occurring at the higher elevations, especially in the Great Smoky and Cumberland mountains. Severe storms are relatively rare because the region lies east of the tornado belt, south and east of the most blizzard occurrences, and too far inland to be much affected by hurricanes (Gale 1985).

The climate of the region may be classified as humid continental. The Cumberland Mountains to the northwest help shield the region from cold air masses that frequently penetrate far south over the plains and prairies in the central United States during the winter months. During the summer, tropical air masses from the south provide warm and humid conditions that often produce thunderstorms. Air stagnation is relatively common in eastern Tennessee. About two multiday air stagnation episodes occur each year, covering an average of about 8 days/year (Korshorver 1982, ORNL 1992).

D.5.1.1.1 Wind directions

In the valleys of ORR, prevailing wind directions [at least to 100 m (330 ft) above ground level] parallel the nearest ridge (ORNL 1992). Because surface wind patterns in the region are determined primarily by topography, slight climatic fluctuations should not alter wind patterns.

D.5.1.1.2 Atmospheric stability and mixing height

Atmospheric stability influences the dispersion rate of contaminants in the atmosphere. Stability for a particular hour is classified in one of seven categories ranging from extremely unstable (A) to extremely stable (G). Because stability is determined largely by the time of day and the large-scale weather features in a region at the time, it tends to be of the same category for a particular hour at all sites of the same elevation in the region. The fact that other climatic parameters related to stability (e.g., temperature and wind speed) have not changed during the period of record indicates that the diurnal and annual distributions of atmospheric stability have not changed (ORNL 1992).

Mixing heights are related to the volume of air through which contaminants may be dispersed. Mixing heights in eastern Tennessee may range from zero (ground-level inversion) to more than 3000 m (9843 ft). The annual average mixing height for the morning is 460 m (1509 ft) and 1541 m (5056 ft) in the afternoon for Anderson County, and the morning and afternoon mixing heights in Roane County are 458 m (1503 ft) and 1543 m (5062 ft), respectively.

D.5.1.1.3 Precipitation

The mean annual precipitation for Oak Ridge is 1356 mm (53.36 in.) (for the years 1964–1993). The maximum precipitation at Oak Ridge in one year was 1939 mm (76.88 in.) in 1973. The maximum precipitation in a 24-hour period was 190 mm (7.48 in) in 1960. The mean number of days with $\geq$ 0.25 mm (0.01 in) precipitation is 129 days (1964–1993). The minimum annual precipitation was 951 mm (37.43 in.) which occurred in 1960 (ATDD 1994).

D.5.1.1.4 Relative humidity

Humidity in eastern Tennessee has not changed appreciably during the last 50 years. Relative humidity in Knoxville averages about 72% (DOC 1989) which is relatively average for the eastern United States. The annual average relative humidity data for Knoxville based on time of day is (ORNL 1992):

- 1 a.m.: 80 %
- 7 a.m.: 85%
- 1 p.m.: 59%
- 7 p.m.: 63%

D.5.1.1.5 Temperature

The mean temperature in Oak Ridge for 1964–1993 ranged between 7.8 C (46.0 F) and 20.2 C (68.3 F) with an average of 14.0 C (57.2 F) (ATDD 1994). The coldest month is January, averaging 2.6C (36.7 F), and the warmest month is July, averaging 24.8 C (76.6F) (DOC 1989a). Extreme temperatures were -27.2 C (-17 F) in January 1985 and 40.6 C (105 F) in July 1952 (DOC 1989a). Temperatures above 32.2 C (90 F) occur

on an average of 31 days/year, with about two-thirds of those days in July and August. Temperatures below freezing occur on an average of 88 days/year, with more than three-fourths of those days in December through February (DOC 1989a).

D.5.1.2 On-site meteorological data

The majority of meteorological data necessary for dispersion modeling of airborne releases is available at the ORR. There are presently three meteorological towers at ORNL, two at the Y-12 Plant, and two at the K-25 Site. Table D.7 summarizes the type of data collected at each meteorological tower. Wind direction, wind speed, and dry bulb temperatures are measured at each height. Other measurements come from the 10-m height, except for rainfall which is collected at approximately 1 m above the ground. The Atmospheric Turbulence and Diffusion Division (ATDD) of the National Oceanic and Atmospheric Turbulence Administration (NOAA) maintains a few meteorological stations in and around ORR and Oak Ridge as well as throughout the region.

Often the meteorological data must be reformatted for dispersion modeling applications. The EPA has developed the Meteorological Processor for Regulatory Models (EPA 1995). This computer program and the associated user's guide are available from the SCRAM BBS. When using meteorological data in dispersion models, it is important that the modeler determine whether the code requires “wind toward” or “wind from” input data; not knowing which data are required could result in serious errors.

D.5.1.3 Worst case impact determination

Establishing the characteristics of a release that provide the upperbound of a potential exposure is what is commonly referred to as determining the “worst-case” impact. Screening programs often require worst-case meteorology. Meteorological conditions that produce the worst dispersion for ground-level releases are those associated with stable atmospheric conditions (F stability) and low wind speeds [1 to 2 meters per second (m/s)]. During daylight hours, the worst case stability is sometimes considered neutral (D stability). For elevated buoyant releases, an unstable atmosphere may result in maximum contaminant concentrations since the plume can be displaced downward resulting in higher ground level concentrations than would occur in a stable atmosphere. For other releases, multiple stability classes and wind speeds need to be modeled to determine the meteorological conditions producing the worst dispersion.

Table D.7. Meteorological data available at the ORR

Site	Tower Name	Collection Height Above Ground (meters)	Initial Data Collection Date[a]	Data Values
ORNL	MT2	10, 30, and 100	1983	Wind direction, sigma theta, wind speed, dry bulb temperature, dewpoint temperature, barometric pressure, solar radiation, and rainfall
ORNL	MT3	10 and 30	1984	Wind direction, sigma theta, windspeed, dry bulb temperature, dewpoint temperature
ORNL	MT4	10 and 30	1984	Wind direction, sigma theta, wind speed, dry bulb temperature, and dewpoint temperature
Y-12	MTE	10, 30, and 100	1987	Wind direction, sigma theta, wind speed, dry bulb temperature, dewpoint temperature, and barometric pressure
Y-12	MTW	10 and 60	1987	Wind direction, signa theta, wind speed, dry bulb temperature, and dewpoint temperature.
K-25	MT1	10 and 60	1985	Wind direction, sigma theta, wind speed, dry bulb temperature, dewpoint temperature, barometric temperature, and rainfall
K-25[b]	MT7	10 and 30	1993	Wind direction, sigma theta, wind speed, dry bulb temperature, dewpoint temperature, barometric pressure, and rainfall

[a] At least a full year of data

[b] K-25 has recently installed six additional 10-m towers and a doplar sonar system

To ensure that meteorological conditions producing worse case dispersion are adequately represented, as many years of representative meteorological data as are available should be modeled; generally, a 5-year period should be adequate (EPA 1995).

D.5.2 Receptor Location

In air dispersion modeling, a receptor can be defined as a point where air concentrations are calculated. The minimum distance to off-site receptors is usually defined by the property boundary or fence line. Realistic receptors should be located at and within a far enough distance from the source to ensure that the maximum concentration is identified.

All "sensitive" receptor locations within a given distance (e.g., 10 km) of the site should be identified. Individual residences and other habitations near the site work areas, schools, day-care centers, and hospitals associated with sensitive population segments, as well as locations where sensitive environmental flora and fauna exist should be located.

Receptors may also be placed at the work areas on-site and at air monitoring station locations. There are multiple emission sources on the ORR; therefore, it may be difficult to ascertain the contribution of a specific remedial activity at the ORR ambient air monitoring stations. For input to a risk assessment, it may also be necessary to place receptors within areas relating to specific exposure pathways, such as waterbodies, dairy farms, and playgrounds.

The receptor grid for an air pathway assessment should be developed on a case-by-case basis in consultation with the resources cited previously in Table D.6. Receptor placement requires special attention when modeling in complex terrain. In addition, to isolate maximum impacts, the emphasis should be placed on receptor resolution and location and not on the total number of receptors modeled (EPA 1995).

Various types of receptor grids can be used. Input of the grid can be based on user specifications, such as desired interval spacing. In general, receptor grids are based on either a polar coordinate or Cartesian coordinate system, or a combination of both systems. In the Cartesian system, the X-axis is positive to the east, and the Y-axis is positive to the north of a user-defined origin. The X and Y coordinates may also be specified in terms of Universal Transverse Mercator (UTM) coordinators, which effectively remove the concept of a grid origin and allow for each receptor to be readily mapped or identified (EPA 1995).

The polar receptor grid is based on radial distances measured from the grid origin and an azimuth bearing (angle) measured clockwise from true north. In the polar coordinate system, receptors are spaced at 22.5-degree intervals in 16 directions on concentric rings.

To establish the location of maximum concentrations, two levels of receptor grids are commonly used in a refined modeling analysis (EPA 1995). A first-level or "screening-level" grid generally comprises a moderate number of receptors located uniformly in all directions from the source. Typically this screening-level grid is centered on a prominent source or feature located within the site boundary. A second-level or "refined" grid comprising receptors more densely located is modeled to pinpoint maximum concentrations based on the results obtained by using the screening-level grid.

D.5.3 Urban/Rural Classifications

For the purpose of dispersion modeling, sites are classified as being either predominantly "urban" or "rural" areas. For the ORR, this determination on future on-site land use is determined through the Common Ground process.

The EPA (1988) provides guidance on appropriate land use classification procedures. In general, the determination of whether the area should be classified as urban or rural begins by estimating the percentages of urban and rural land use types that occur within 3 km of the site. Table D.8 lists common land use types and their urban or rural designation. If land use types I1, I2, C1, R2, and R3 account for 50% or more of the total area (within 3 km of the source), then the site is classified as urban for modeling purposes; otherwise, it is classified as rural.

D.5.4 Averaging Time Considerations

Several averaging periods may be of interest for any given analysis, including instantaneous, 15-minute, 1-hour, 24-hour, monthly, and annual. The averaging periods to evaluate will depend on the time periods of the applicable action levels. The choice of time periods will also depend on the specific compounds present and their associated health effects.

Several categories of action levels may be necessary, depending on the compounds of interest, the operating life of the source, the type of emission sources, and the potentially affected population. Categories of action levels used most often are long-term (annual) action levels for carcinogens and noncarcinogens and short-term action levels for acute toxins.

To derive impacts for averaging periods, such as 3-hour, 8-hour, 24-hour, annual screening-level models such as TSCREEN, one should use time scaling factors. These scaling factors account for the variability in meteorological conditions that may occur over a longer time period. Concentrations for various avenging periods can be automatically calculated with refined models, given their use of site-specific meteorological data.

D.5.5 Exposure Pathway Parameters

All of the air dispersion models for radionuclides have exposure pathway assessment capabilities. None of the chemical contaminant models, except MEPAS, have an exposure assessment component. Many of the radionuclide codes were developed to assess doses to off-site receptors at specific sites (i.e., Hanford) or for specific applications [i.e., National Emissions Standards for Hazardous Air Pollutants (NESHAP) compliance]. Therefore, the default exposure pathway parameter values provided in these codes may be different from the EPA's *Risk Assessment Guidance for Superfund* (RAGS) (1989) exposure pathway parameter values. For example, as shown in Table D.9, the human consumption rates in CAP-88 PC and GENII-S are not the same (GENII exposure pathway parameters values are specific to Hanford applications) nor are these values similar to those specified as default in MEPAS or recommended in RAGS. Where possible, site-specific parameter values should be used.

Table D.8. Classification of land use types

Type	Description	Urban or Rural
I1	Heavy Industrial	Urban
I2	Light/Moderate Industrial	Urban
C1	Commercial	Urban
R1	Common Residential (Normal Easements)	Rural
R2	Compact Residential (Single Family)	Urban
R3	Compact Residential (Multi-family)	Urban
R4	Estate Residential (Multi-acre Plots)	Rural
A1	Metropolitan Natural	Rural
A2	Agricultural	Rural
A3	Undeveloped (Grasses/weeds)	Rural
A4	Undeveloped (Heavily wooded)	Rural
A5	Water Surfaces	Rural

Sources: (EPA 1986, 1995)

Table D.9. Human consumption rates for general population

Input	CAP88-PC	GENII	GENII-S	MEPAS	RAGS	Reg. Guide 1.109
Leafy Vegetables (Kg/yr)	18	15	15	73.0 total with non-leafy	73 total with non-leafy	
Non-leafy Vegetables (Kg/yr)	176	140	140	73.0 total with leafy	73 total with leafy	Total of 190
Fruits (Kg/yr)	N/A	64	64		51.1	
Cereals (Kg/yr)	N/A	72	72			
Cow Milk	112 L/yr	230 Kg/yr	230 Kg/yr	Age 1- 6: 186 Kg/yr Other Ages: 111 Kg/yr	Fat & Dairy = 24-43 g/day; Fresh Milk = 10.7 g/day ave	110 L/yr
Meat (Kg/yr)	85	70	70	For Beef Only: 27.4	Beef: 0.28 Kg/meal or 15-26 g/day	Total of 95 with Poultry
Poultry (Kg/yr)		8.5	8.5			Total of 95 with Meat
Eggs (Kg/yr)	N/A	20	20		0.15 Kg/meal	N/A
Fish (Kg/yr)	N/A	6.9	6.9		2.4	6.9
Drinking Water	N/A	440 Kg/yr	440 Kg/yr	Resdt'l: 2 L/day Commc'l: 1 L/day	Resdt'l: 2 L/day Commc'l: 1 L/day 1.4 L/da (ave)	370
oil Sediment (mg/day)						
Res/Land Use	N/A	N/A	N/A	Age 1 to 6 = 200 Other Ages = 100	Age 1 to 6 = 200 Other Ages = 100	
Com'l/Ind'l.				Adult Worker = 50	Adult Worker = 50	

Table D.6 identifies a few ORR resources for this information. As shown in Table D.9, the modeler needs to be aware of the differences in exposure pathway parameter values (and definitions) between the codes and

RAGS documentation.

D.6. MODEL UNCERTAINTY

The accuracy of model estimates varies with the model used, the type of application, and site-specific characteristics. EPA studies of model accuracy have confirmed that models are more reliable for estimating longer time-averaged concentrations than for estimating short-term concentrations at specific locations and that models are reasonably reliable in estimating the magnitude of highest concentration occurring sometime, somewhere within an area (EPA 1978). For example, errors in highest estimated concentrations of $\pm$ 10% to 40% are typical for many of the models (EPA 1995). However, estimates of concentrations that occur at a specific time and site are poorly correlated with actually observed concentrations and are much less reliable (EPA 1995).

Some of the codes, e.g., GENII-S, RESRAD, MEPAS, have the capability to conduct uncertainty analyses (see Sect. D.5). However, the technical information on how to measure model uncertainty is incomplete; no specific guidance on the consideration of model uncertainty is presently available (EPA 1995). In the meantime, it is acceptable to consider model results as a "best estimate" (EPA 1995).

D.7. CONCLUSIONS

The purpose of this report is to provide technical guidance for atmospheric dispersion modeling to contractors conducting baseline studies and FSs at ORR CERCLA sites. In addition, it provides a summary of approaches for source term characterization, tools for selecting appropriate models for specific risk assessment applications, resources for site-specific data, and references for additional information.

For screening and refined routine air dispersion analyses for radionuclides, COMPLY, CAP88-PC, and GENII are applicable. For nonroutine analyses, Hotspot and RASCAL would be applicable. TSCREEN is a useful chemical contaminant screening model; for refined modeling, ISC3 is recommended by the EPA. If ISC3 is not available, PAL is recommended for assessing area sources. MEPAS is the only code currently that can assess both radionuclide and chemical contaminants. However, the other codes may be very useful for a particular situation.

Modelers must understand the strengths and limitations of a model before applying it to a specific situation. Model application should proceed only after the modeler understands the technical formulation, features, and assumptions incorporated into the model. If there are questions concerning the use of a particular code, contact those resources specifically knowledgeable of the code attributes. For additional literature, refer to the references and Appendix B. For specific information on codes contact the EPA OQAPS organization, and for site-specific data, refer to those resources identified in Table D.6.

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D.9 EMISSION RATES

Table D.10. Summary of baseline emission rate methods

Type of Emission	Media	Measurements	Predictive[a]
Gaseous Emissions	Subsurface Soils	Soil Gas measurements are preferred $Ei = \frac{(Di*Ci*A\ (P_r^{4/3})}{d_{sc}}$	If use soil bulk concentrations $C_{sat}=(K_d*s*n_m)+(s*0_m)$ Eqn: RAGS Volume 1 Section 3.31 Oct 1991, (pg8)
Gaseous Emissions	Nonaerated Surface Impoundments and Contaminants (In solution)Pooled at Soil Surfaces	Measure liquid phase concentrations	Using liquid phase concentrations calculate ER: $E_i = K_i*C_s*A$ Ref: EPA-450/3-84-020
Volatile Nonmethane Organic Compound (NMOC)	Codisposal in Landfills	Measure soil gas concentrations	Using measured soil gas concentrations Emission rate for each volatile NMOC: $E_i = C_i*V_y*A$ Ref: EPA-450/1-92-002
Free-Phase Volatile Contaminants	Directly into Atmosphere (open drums/containers, fresh spills, etc.,where free product exists)	For any and all free-phase volatile contaminants directly exposed to atmosphere an in-depth APA is warranted. Source monitoring is recommended for emissions rates.	Use measured source emission rates with refined modeling Or use ambient air monitoring results
Solid and Semivolatiles	Adsorbed onto fugitive dust	Measure contaminant-specific bulk concentrations of erodible surface materials.	Wind erosion -- 2 types of emission flux (g/m2-h) models: Unlimited Reservoir: $E_{10}= 0.036\ (1-V)([u]^3/u_t)^3\ F(x)C$ Limited Reservoir: $E_{10} = 0.83\ \{(f)*P(u^+)*(1-V)*(C)/(1000*(PE/50)^2\}$ Total Emission Rate (g/s) $E^T = (E_x*A)/3600$ Ref: EPA-600/8-85/002

[a]See following page for term definition

Source: (EPA 1992)

Table D.10. Baseline emission rate terms

Soil Gas Measurements -- Subsurface soils

E_i	=	emission rate of component i, g/s
D_i	=	diffusion coefficient of component i air, cm^2/s
C_i	=	vapor concentration of component i measured in the soil pore spaces, g/cm^3
A	=	exposed surface area, cm^2
P_t	=	Total soil porosity, dimensionless. P_t assumes dry soil (worst-case); if soil is wet more often than dry, substitute the term $(Pa^{10/3}/P_t^2)$ for the term $P_t^{4/3}$
d_{sc}	=	Effective depth of soil cover, cm
C_{sat}	=	Saturation concentrations, mg/kg (ppm)
K_d	=	Soil/water partition coefficient, l/kg (or ml/g)
s	=	solubility of contaminant in water, mg/l-water
n_m	=	soil moisture content expressed as a weight fraction, kg-water/kg-soil
$_m$	=	soil moisture content, l-water/kg-soil (or ml/g)

Volatile Nonmethane Organic Compound (NMOC)

C_s	=	liquid-phase concentration of component i, g/cm^3
K_i	=	overall mass transfer coefficient, cm/s
V_y	=	mean landfill gas velocity in the soil pore spaces, cm/s

Solid and Semivolatiles

E_{10}	=	PM_{10} annual average emission flux of component i, g/m^2-h
V	=	Fraction of contaminated surface with continuous vegetative cover (equals 0 for bare soil)
[u]	=	mean annual windspeed at 10 m anemometer height, m/s (from local climatological data)
u_t	=	equivalent threshold value of windspeed at 7 m anemometer height, m/s
C	=	Fractional percent by weight of component i from bulk samples of surface material
F(x)	=	Function obtained from the relationship in threshold friction velocity
$P(u^+)$	=	erosion potential, i.e., quantity of erodible particles at the surface prior to the onset of erosion, g/m^2
f	=	frequency of disturbances per month (1/month for abandoned sites or sites with no activity)
PE	=	Thornwaite's Precipitation-Evaporation Index used as a measured soil moisture content

Table D.11. Default emission rates and methods for estimating emission rates for typical remedial technologies

Technology	Pollutant	Default Emission Rates (g/hr)		Methods for Estimating Emission Rates[a]	References
		Controlled	Uncontrolled		
Excavation	VOC	15	70	$ER = (S_v * C * b * 1)/(t_{R)}$	EPA-450/1-92-004
Rotary kiln incineration	VOC PM_{10}	340 4,260	340 695,000	ER = FR * (1 - DRE/100) * (0.126) for VOCs $ER = (0.08 * Q_G * 0.00108)$ for particulate	EPA-450/1-92-003
Infrared incineration	VOC PM_{10}	10 16.2	10 0.6-29	$ER_i = (1 - (DRE\ i/100)) * C_i * m_w$	EPA-450/1-91-001
Air stripping Small unit Medium unit Large unit	VOC VOC VOC	342 1704 3420	3420 17040 34200	$ER = C_i * L_R * (SE_i/100) * (1-\%CE_i/100) *$ (0.06) controlled $ER = C_i * L_R * (SE_i/100)*$ (0.06) uncontrolled	EPA-450/1-91-001
Soil vapor extraction	VOC	1250	25,000	$E_i = R_{l,i} * (1 -(\%CE_{l,i}/100)) + R_{v,i} * (1 - (\%Ce_{l,i}/100))$	EPA-450/1-91-001
Solidification and stabilization	VOC	N/A	5460	$ER_i = C_i * M * (\%V_i/100)$	EPA-450/1-91-001
Ultrox oxidation	VOC	N/A	4.5	$E_i = C_i * V * (R_{eff}/100) * (T_{frac}/100)* (1 - \%CE_{i}/100)$ or $E_i = C_i * V * (1 - R_{eff}/100)$ for byproducts	EPA-450/1-91-001
Flow-through treatment with mechanical aeration	VOC	N/A	4800	$ER_{i =} (C_i/1000) * V * (\%V_i/100)$	EPA-450/1-91-001
Quiescent flow-through treatment	VOC	N/A	720	$Er_{i =} (C_i/1000) * V * (\%V_i/100)$	EPA-450/1-91-001
Disposal impoundments	VOC	N/A	48.6	$ER_i = (C_i/100) * V * (\%V_i/100)/(t)$	EPA-450/1-91-001

[a] Refer to following page for term definition

Table D.11. Remedial technologies term definition

ER_i	=	emission rate for contaminant "i" (g/s)
E_i	=	emission factor for contaminant "i" (g/hr)
FR	=	feed rate (lb/hr)
V	=	volume flowrate of soil or water being treated (m^3/hr)
R_{eff}	=	overall removal efficiency of treatment technology (%)
T_{frac}	=	fraction of removed contaminant transferred to air (%)
DRE	=	destruction and removal efficiency
Q_g	=	gas flow rate
C_i	=	concentration of contaminant in influent water (mg/L) or contaminated soil (g/kg)
b	=	bulk density of soil (g/cm^3)
t_R	=	duration of remediation (s)
L_R	=	influent liquid flowrate (L/min)
M	=	mass rate of soil treated
V_i	=	percentage of contaminant "i" volatilized
SE	=	stripping efficiency (%)
S_v	=	volume of contaminated soil (m^3)
%CE	=	control efficiency of stripper exhaust treatment (%)
$R_{l,i}$	=	removal rate of contaminant "i" in liquid phase (g/hr)
$R_{v,i}$	=	removal rate of contaminant "i" in vapor phase (g/hr)
$\%CE_{l,i}$	=	% control efficiency of liquid treatment device
$\%CE_{v,i}$	=	% control efficiency of vapor treatment device
m_w	=	total mass flow rate of waste feed (kg/hr)

Table D.12. Particulate (15 µm) and VOC emission rates from soils handling

Technology	Particulate Emission Rate (kg/hr)	VOC Emission Rate (kg/hr)	
		Controlled	Uncontrolled
Excavation	2	0.015	0.07
Soil Transport	15	0	0.63
Dumping	0.16	0.152	5.1
Grading[a]	4.1	0.152	5.1

Source: EPA 1989b.

[a] Grading is not expected to increase VOC emissions if performed soon after dumping, so grading ER = dumping ER.

Table D.13. Particulate emission rates for incineration

Technology	Estimated Emission Rates (g/hr)	
	Controlled	Uncontrolled
Rotary kiln incineration	4,260	695,000
Infrared incineration	16.2	0.6–2.9

Source: EPA 1991a.

Table D.14. VOC emission rates for typical treatment technologies

Technology	Pollutant	Estimated Emission Rates (g/hr)	
		Controlled	Uncontrolled
THERMAL TREATMENT:			
Rotary kiln incineration[a]	VOC	340	340
	Metals	170	170
	HCl	1.4	140
	HF	0.4	40
	SO_2	17	340
	CO	3,510	3,510
	NO_x	11,530	11,530
Infrared incineration	VOC	10	10
	Metals	5	5
	HCl	0.041	4.1
	HF	0.011	1.1
	SO_2	0.5	10
	CO	2.7	2.7
	NO_x	16	16
Air stripping[b]	VOC	342	3420
Soil vapor extraction	VOC	1,250	25,000
Solidification and stabilization	VOC	NA	5460
PHYSICAL AND CHEMICAL TREATMENT METHODS:			
Ultrox oxidation	VOC	NA	4.5
BIOTREATMENT AND LAND TREATMENT:			
Flow-through treatment with mechanical aeration	VOC	NA	4800
Quiescent flow-through treatment	VOC	NA	720
Disposal impoundments	VOC	NA	48.6

Source: EPA 1991a.

a Based on a typical incinerator with heat load of 63 MM kilojoules/hr, waste feed of 3400 g/hr, and stack gas flow of 986 m^3/min.

b Air stripping values are for small units; for medium and large units, values increase by a factor of 10 for each size increase.

D.10 COMPENDIUM OF AIR/SUPERFUND PROGRAM DOCUMENTS

Title	EPA and NTIS No.	Date
Volume 1 -- Overview of Air Pathway Assessments for Superfund Sites (Revised)	EPA-450/1-89-001a NTIS PB93-173987	11/92
Volume II -- Estimation of Baseline Air Emissions at Superfund Sites	EPA-450/1-89-002a NTIS PB90-270588	8/90
Volume III -- Estimation of Air Emissions Emissions form Clean-up Activities at Superfund Sites	EPA-450/1-89-003 NTIS PB89-180061/AS	1/89
Volume IV -- Guidance for Ambient Air Monitoring at Superfund Site (Revised)	EPA-451/R-93-007 NTIS PB93-199214	5/93
Volume V -- Procedures for Air Dispersion Modeling at Superfund Sites	EPA-454/R-95-003	2/95
A Workbook of Screening Techniques for Assessing Impacts of Toxic Air Pollutants	EPA-450/4-88-009 NTIS PB89-134340	9/88
Area Source Dispersion Algorithms for Emissions Sources at Superfund Sites	EPA-450/4-89-020 NTIS PB90-142753	11/89
Users Guide to TSCREEN - A Model for Screening Toxic Air Pollutant Concentrations	EPA-450/4-90-013 NTIS PB91-141820	12/90
User's Guide for the Fugitive Dust Model	EPA-910/9-88-202R NTIS PB90-215203	1/91
Emission Factors for Superfund Remediation Technologies	EPA-450/1-91-001 NTIS PB91-190-975	3/91
Estimation of Air Impacts for Air Stripping of Contaminated Water	EPA-450/1-91-002 NTIS PB91-211888	5/91
Database of Emission Rate Measurement Projects (Technical Note)	EPA-450/1-91-003 NTIS PB91-222059LDL	6/91
Guideline for Predictive Baseline Emissions Estimation Procedures for Superfund	EPA-450/1-92-002	1/92 (In revision)
Estimation of Air Impacts for Soil Vapor Extraction (SVE) Systems	EPA-450/1-92-001 NTIS PB92-143676/AS	1/92
Screening Procedures for Estimating the Air Impacts of Incineration at Superfund Sites	EPA-450/1-92-003 NTIS PB92-171917	2/92

Title	EPA and NTIS No.	Date
Estimation of Air Impacts for the Excavation of Contaminated Soil	EPA-450/1-92-004 NTIS PB92-171925	3/92
Assessing Potential Indoor Air Impacts for Impacts for Superfund Sites	EPA-451/R-92-002 NTIS PB93-122257	9/92
Air Emissions from Area Sources: Estimating Soil and Soil-Gas Sample Number Requirements	EPA-451/R-93-002 NTIS PB93-173995	3/93
Models for Estimating Air Emission Rates from Superfund Remedial Actions	EPA-451/R-93-001 NTIS PB93-186807	3/93
Estimation of Air Impacts from Area Sources of Particulate Matter Emissions at Superfund	EPA-451/R-93-004 NTIS PB93-215648	4/93
Estimation of Air Impacts for Bioventing Systems Used at Superfund Sites	EPA-451/R-93-003 NTIS PB93-215655	4/93
Estimation of Air Impacts for Solidification and Stabilization Processes Used at Superfund Sites	EPA-451/R-93-006 NTIS PB93-215622	4/93
Estimation of Air Impacts for Thermal Desorption Units Used at Superfund Sites	EPA-451/R-93-005 NTIS PB93-215630	4/93
Rapid Assessment of Exposure to Particulate Emissions from Surface Contaminations Sites	EPA/600/8-85/002 NTIS PB85-192219	2/85
Superfund Exposure Assessment Manual Superfund Sites	EPA/540/1-88/001 PB89-135859	4/88
Compilation of Air Pollutant Emission Factors Volume I: Stationary Point and Area Sources Volume II: Mobile Sources	AP-42 PB86-124906 PB87-205266	 9/85 (later date revisions) 9/85

APPENDIX E

GUIDE FOR GROUNDWATER MODELING FOR RISK ASSESSMENT

E.1 INTRODUCTION

As one of the primary data users in the Remedial Investigation/Feasibility Study (RI/FS) process, risk assessors often rely on models to characterize site conditions when existing data are not adequate or to predict future potential exposures. As a result, models have become an essential tool to supplement extant data. Although numerous United States Environmental Protection Agency (EPA) and United States Department of Energy (DOE) documents provide guidance for the development of data quality objectives (DQO), the use of data in risk assessments, and the role of risk assessment in the RI/FS process, minimal guidance is provided on the selection and use of models to support risk assessment activities. Therefore, it is essential that the selection of groundwater models for risk assessment be integrated into the planning stages of the RI. If the basic model selection process is incorporated into the existing DQO framework, then modeling quality, data quality, and thereby risk assessment quality would be improved.

EPA has adopted the DQO process as a means of scoping data needs and limits on uncertainty for RIs. Because these guidelines have been established, modeling objectives can be developed and contributed to the existing framework to encourage appropriate and technically defensible modeling decisions during the risk assessment process. Once the model selection process is defined in its relationship to the DQO process, critical decision points and data gaps with respect to modeling can be identified, and uncertainties associated with modeling can be reduced or, at least, defined. A standard approach to the selection of models in risk assessment is critical to developing consistent, rational interpretations of risk estimates and assessing the need for or most efficient manner of performing remediation.

Currently, model selection is not specifically an integral part of the DQO process. If the model selection process were standardized, project team members would have a better understanding of how modeling decisions are intimately tied to data quality issues and uncertainty issues in risk assessment. Increased communication and interaction among modelers, risk assessors, hydrogeologists, and the rest of the RI team would be encouraged by this interdependency for reducing the uncertainty associated with the investigation. Consequently, more intelligent decisions could be made regarding what model is best suited for the risk assessment, and more of the uncertainties involved in risk assessment could be quantified and appropriately managed.

The purpose of this document is to provide guidance on a standard approach to model selection for the Oak Ridge Reservation and define the relationship of model selection to the DQO process. If one of the objectives of modeling is to reduce the level of uncertainty associated with risk assessment and remedial decisions, then the consequences of selecting a simple model over a complex model or vice versa must be identified. Finally, examples of the importance of applying the model selection process are provided. The ultimate objective of these discussions is to provide information that will assist in understanding uncertainties associated with modeling and the consequences of those uncertainties on the risk assessment and subsequently the remedial action.

E.2 THE FRAMEWORK FOR MODEL SELECTION

The RI/FS is a phased, iterative process. Data are generally collected in several stages. As a basic understanding of site characteristics is achieved, subsequent data collection efforts focus on filling identified data gaps for risk assessment and gathering information necessary to evaluate remedial alternatives. This phased sampling approach encourages identification of key data needs as early in the process as possible to ensure that data collection is always directed toward providing information relevant to the risk assessment and

selection of a remedial alternative. In this way, the overall site characterization effort can continue to be scoped to minimize the collection of unnecessary data and maximize data quality. Scoping is the initial planning phase of the RI/FS process, and many of the planning steps begun at this stage are continued and refined in later phases of the RI/FS.

The main objectives of scoping are to identify the types of decisions that need to be made, determine the types (including quantity and quality) of data needed, and design efficient strategies to collect these data. Currently, decisions regarding modeling tend to be made independently of data collection efforts, when in actuality modeling goals may have a direct impact on data needs. Modeling requirements, like data quality and risk assessment considerations, must be assessed early, during scoping, to ensure that data are collected to support DQOs, modeling objectives, and risk assessment objectives. The selected modeling approach should not be driven by the data availability, but by the objectives, which should be defined in terms of the decisions that must be made and the level of certainty required to make those decisions.

The DQO process is the framework that has been adopted by EPA to ensure that appropriate steps are taken to plan for and implement an effective investigation. Potential site-specific modeling decisions should be made in association with DQO decisions to ensure that models chosen will supplement the sampling data and effectively support risk assessment activities. A preliminary site modeling strategy developed concurrently with the DQO process would allow model input requirements to be incorporated into the data collection requirements.

Modeling may entail something as simple as a qualitative estimate, to mass balance calculations, to a complex three-dimensional flow and transport model. In any case, a model is a tool used to bracket uncertainty associated with not collecting certain data, help refine the conceptual site model and understand site conditions; and predict concentrations and risk in the future under no action and various remedial action scenarios. By defining the questions that need to be answered using modeling as a tool, the most appropriate model can be selected based on what tool can answer the question best. The RI team can also decide if the level of uncertainty associated with not collecting the data is of sufficient magnitude to warrant the cost of collecting the data.

A standard approach to model selection can encourage the documentation of how and why a particular model was chosen, which would allow a more accurate interpretation and use of models and results. For example, frequently, risk assessment models are chosen based on their ability to provide conservative estimates of groundwater movement and contaminant concentrations (i.e., the results provide the fastest migration and the greatest contaminant concentrations that could occur at an exposure point). This application will result in an upperbound estimate of the potential risk. However, if the same modeling scenario were used to predict clean-up time and costs, both would likely be underestimated due to the fact that the original purpose of the model was to conservatively estimate contaminant migration. Actual migration may occur at a much slower rate, resulting in a longer and more costly cleanup than predicted by the model. In this case, although it may appear that time and money were saved by applying the same model in the same way for two questions, an erroneous prediction was used to make critical clean-up decisions.

For proper scoping to occur, risk assessors, experienced modelers, hydrogeologists, and project managers must all play an integral part in the RI/FS planning process. This involvement will ensure that adequate environmental analytical data of acceptable quality are collected and that appropriate and defensible modeling decisions are made during the RI/FS. Risk assessors and modelers should work closely to identify and recommend models that will maximize the quality of the baseline risk assessment within the site related and budgetary constraints of the RI/FS and will produce consistent results useful to risk managers in making

remedial decisions.

Establishing a relationship between the model selection process and the DQO process is the first step toward developing an approach to model selection. The following subsections describe the DQO process, the proposed model selection process, and their interactive relationship.

E.2.1 The Data Quality Objectives Process

The DQO process is a management tool used to develop a scientific and resource-effective sampling design. DQOs are qualitative and quantitative statements derived from the output of each step of the DQO process that:

- clarify the study objective,
- define the most appropriate type of data to collect,
- determine the most appropriate conditions from which to collect data, and
- specify acceptance levels of decision errors that will be used as the basis for establishing the quantity and quality of data needed to support the decision.

DQOs must strike a balance between time, money, and data quality. The DQO process must be initiated during project planning to produce work plans resulting in data having a quantifiable degree of certainty. The end use of data to be collected, quality of data required, and cost to produce data will determine required DQOs.

The first step in initiating any significant environmental data collection program should be the development of DQOs. DQOs help to define the purposes for which environmental data will be used and set guidelines for designing a data collection program. DQOs are used to define quality assurance/quality control programs specifically tailored to the data collection program being initiated.

The DQO process consists of seven steps. In most cases, each successive step derives information from the previous ones; therefore, each step should be completed in the order shown. The DQO process is iterative, however, so it may be useful to refine the outputs from previous steps. Iteration is encouraged since it leads to a more focused study with a greater chance of meeting its objectives. Above all, every step should be completed before data collection begins. The purpose of each step of the DQO process is described in Table E.1. For more information on the DQO process, refer to *Guidance for the Data Quality Objectives Process* (EPA QA/G-4, 1994).

Table E.1. Purpose of DQOs steps

Data Quality Objectives Step	Purpose
Step 1: State the Problem	To clearly define the problem that requires new environmental data, so the focus of the study will be clear and unambiguous.
Step 2: Identify the Decision	To define the decisions that will be resolved using data to address the problem.
Step 3: Identify Inputs to the Decision	To identify the informational inputs that will be required to resolve the decision and determine which inputs require environmental measurements.
Step 4: Define Boundaries of the Study	To specify spatial and temporal circumstances covered by the decision.
Step 5: Develop a Decision Rule	To integrate outputs from previous steps into a single statement that describes the logical basis for choosing alternative actions.
Step 6: Specify Limits on Decision Errors	To specify the decision maker's acceptance limits on decision errors, which are used to establish appropriate performance goals for limiting uncertainty in the data.
Step 7: Optimize the Design	To identify the most resource effective sampling and analysis design for generating data expected to satisfy DQOs.

E.2.2 The Model Selection Process

The model selection process is not entirely separate from the DQO process but is complementary and concurrent with DQO development. The basic steps of the model selection process will be described in this section, and the relationship between the processes will be described in the following section.

The model selection process is a management tool used to develop scientific and resource-effective modeling options. To develop these options, appropriate modeling goals must be defined and refined through an iterative process from problem identification through model application. Figure E.1 displays the model selection process, and Table E.2 shows the purpose of each step in the process. Interaction among risk assessors, hydrogeologists, modelers, and the rest of the project team is the most important factor in production of a cohesive plan for data collection that will address conceptual site model data gaps and modeling data gaps through the same effort.

Table E.2. Purpose of model selection steps

Model Selection Step	Purpose
Step 1: Problem Identification	To define the site problem in terms of potential risk or potential remediation to be considered.
Step 2: Compile and review existing data	To develop a site description and gather information for the conceptual site model.
Step 3: Develop conceptual site model	To develop a conceptual site model that integrates hydrogeological and risk assessment focuses.
Step 4: Identify gaps in the conceptual site model	To identify gaps in knowledge of the conceptual site model that either data or modeling may be able to address.
Step 5: Determine what key questions and data gaps should be addressed with modeling	To identify the need for modeling and refine the statement of the problem.
Step 6: Identify modeling goals	To identify the questions that need to be answered by any modeling effort.
Step 7: Identify boundaries on resources and uncertainties	To determine the constraints under which any modeling effort must operate; to put bounds on the level of uncertainty that is acceptable for any modeling effort.
Step 8: Evaluate tools	To evaluate critical inputs and outputs of potential models; to determine data needs based on critical inputs and outputs.
Step 9: Provide DQO team with potential modeling scenarios	To provide descriptions of all models that could address the modeling goals; to describe the advantages and disadvantages of each modeling option with regard to previously determined boundaries on resources and uncertainties; may conduct preliminary sensitivity analysis to assess impact of input uncertainties on predictions.
Step 10: Determine data to be gathered	To combine all information from the model selection process and the DQO process and decide what data will fulfill all requirements to meet the agreed upon objectives for the investigation.
Step 11: Select model	To select the most appropriate model based on the optimum combination of goals and boundaries.
Step 12: Gather data and run model option	To fulfill the modeling and data objectives to refine the conceptual site model to make technically defensible risk management decisions.
Step 13: Conduct sensitivity analysis and uncertainty analysis	To determine what parameters affect the modeling results the most in an effort to identify areas of uncertainty and assist in the next iteration of data collection decisions.

E.2.3 The Relationship Between the Model Selection Process and the Data Quality Objectives Process

The DQO process and the model selection process are complementary and interdependent strategies for decision-making. Because one of the major goals of the DQO process is to define the purpose for which environmental data will be used, it is essential that the model selection process be performed concurrently with the DQO process and that the RI/FS team be interactive throughout both processes. Specific points in the DQO process require information from the model selection process to appropriately assess data needs. For example, if soil contamination concentration data are going to be collected, it may be critical to predictive modeling of future risk from leaching that information on percent organic carbon content, permeability, grain size distribution, water content, and/or recharge rate be collected. As stated previously, every step of the DQO process should be completed before data collection begins. In addition, the model selection process should be completed at the same level and with the same iteration as the DQO process. The establishment of a dynamic

relationship among team members involved in these processes can only occur with an understanding of the importance of the full application of the model selection process.

A standard approach to model selection does not imply that modeling decisions can be made in a cookbook fashion. For example, a screening level model may appear to be appropriate for a number of sites at a facility based on scoping information. If the data at a particular site indicate that more complicated processes are involved, it may be necessary to select another model for this individual site if the processes involved may have a significant effect on contaminant transport. Accordingly, during the initial phases of a remedial project, and throughout the remedial process, the remediation manager must continually assess the need to employ models to answer specific risk assessment and remedial action questions. The level of intensity or complexity of model selection and the models used are heavily influenced by the phase of the RI/FS, the level of acceptable uncertainty, and available resources.

E.2.3.1 Purposes of modeling

The purpose of modeling in risk assessment is to refine the conceptual site model and reduce uncertainty so that remedial decisions can be made. One should generally begin with the simplest model that will satisfy the objectives and progress toward the more sophisticated codes until modeling objectives are met. The remedial process is generally structured in a manner that is consistent with this approach (i.e., as the investigation proceeds, additional data become available to support more sophisticated groundwater modeling). Scoping, site characterization, and the remedial phase of the RI/FS process each have varying levels of data for model application and should have varying levels of modeling goals. Model quality cannot exceed data quality. As more data collection is planned, it is essential that the DQO process result in DQOs that consider the data needed to fulfill modeling objectives. The marriage of these processes is a quality assurance measure that will ensure the collection of data to support project objectives rather than the derivation of objectives based on limited available data or modeling.

The following subsections will provide details on the relationship of the model selection process to the DQO process. The model selection process will be the framework for discussion, and the critical points of input from or output to the DQO process will be specified.

E.2.3.2 Problem identification

Problem identification involves the preliminary definition of potential risk or remediation questions that should be considered. At the scoping phase of the project, the question may be as simple as “Is contamination present at the site?”. This question becomes more refined as the process is reiterated. Subsequent iterations may question “How long will it take for contaminant ‘x’ to reach a residential well at concentrations above risk levels?”. An FS question might be “Will this specific remedial action result in risk reduction?”. The initial problem identification will help to establish the level of intensity of the investigation as a scoping or characterization exercise. It should be noted that the first step of the DQO process is also a statement of the problem. This fact illustrates the need for early communication among team members to focus on a common goal or questions to be resolved.

E.2.3.3 Compile and review existing data

Each project and phase of the RI/FS will have varying levels of available data. All data related to the site should be reviewed, including previous risk calculations and modeling attempts. It may also be appropriate to

review information from other similar sites or projects. The quality of the data and previously used models will be an indication of the current level of uncertainty associated with available information. Without knowledge concerning the uncertainty associated with site information, decisions are essentially being made on a random basis. Review of prior DQOs and modeling goals will reveal how and what goals have been achieved in the past, as well as the focus of past site investigations.

E.2.3.4 Develop a conceptual site model

Based on the data and modeling results reviewed in the previous step, a hydrogeological conceptual site model is developed. This model should indicate the level of certainty associated with each assumption, so it can be correctly interpreted. Risk assessors also will have performed these steps resulting in a conceptual site model that focuses on exposure pathways and points of receptor contact. The hydrogeological conceptual site model and the risk assessment conceptual site model must be integrated if they are to be complementary. For example, the risk assessor may be concerned with administrative boundaries based on the location of a residential receptor's home, while the groundwater modeler's conceptual site model may be focused on hydrogeologic boundaries on a regional scale. In other cases, the risk assessor may not consider an important hydrogeological process that must be characterized to predict contaminant concentrations at the receptor exposure point. The team must communicate during the development of the conceptual site model to ensure all technical personnel are focused on answering pertinent questions about risk and remediation.

E.2.3.5 Identify conceptual site model data gaps and key questions

After available data have been assessed relative to the site problem, gaps and uncertainties in the data are found. The entire RI/FS team, including modelers, risk assessors, hydrogeologists, etc., should be involved in the identification of data gaps. In addition, for each data gap, the consequences of not filling the data gap should be discussed in terms of defining potential uncertainties. At this point in the process, it may be possible to further refine the statement of the problem into key questions. For example, by building the conceptual site model based on both hydrogeological principles and risk assessment principles, it is determined that measurement of a particular parameter is necessary to assess risk to a receptor of groundwater contamination. The question becomes refined from "Is the receptor at risk?" to "What is the site-specific flow rate?" so that modeling can occur. However, it may be determined that modeling is not needed to answer the key questions of this iteration of the process; in this case, the decision not to model may follow.

E.2.3.6 Identify boundaries on resources and uncertainties

Every project has limitations with regard to time, budget, personnel, and available tools. As a result of these constraints, all uncertainties cannot be addressed or reduced. The goal is to design a sampling and modeling plan that optimizes resources to reduce uncertainties to the greatest extent possible. All project personnel should be involved in defining the boundaries of the study to ensure focus on a common and pertinent question. Each professional brings a valuable perspective to the success of data collection, modeling efforts, risk characterization, and remediation. The output of this step is a defined schedule and budget, as well as defined levels of acceptable uncertainty to make decisions.

E.2.3.7 Identify modeling goals

The identification of key questions, data gaps, and constraints within which the investigators must operate serves to create the atmosphere in which modeling goals must be developed and helps focus efforts on project

objectives. An important question to ask at this point is, “Can purposeful modeling goals be developed within this atmosphere?”. If the answer is no, it may be that modeling is not a viable option for reducing site uncertainty. In addition, the modeling goals should be in line with the phase of investigation and iteration of the model selection and DQO processes. The goal of modeling is heavily influenced by the phase of the RI/FS process being performed. In all cases, the uncertainties that will be reduced by achieving the modeling goals should be identified. These goals should be a determining factor in the DQO process as to what data will be collected and what quality assurance will be performed.

E.2.3.8 Evaluate potential models

To evaluate potential models to be used in support of the investigation, the team must also examine critical processes in the conceptual site model and data gaps specific to each model.

Identify critical processes to be modeled. Many incorrect predictions in modeling may be attributable to including or excluding specific flow and transport processes. The modeler must decide what processes are critical to the modeling effort in terms of how much uncertainty will be involved if the process is ignored. Some typical modeling processes that may have an impact if not considered are:

- discrete fracture flow and transport;
- “storm flow zone” flow and transport;
- karst features or conduits;
- matrix diffusion-retardation effects on contaminant transport;
- differing geochemical processes in regolith, shales, and carbonate that result in different transport rates for different contaminants (e.g., inorganics, VOCs, and radionuclides); and
- rapid flushing in the shallow zone with discharge to local tributaries.

If these processes are involved, it does not necessarily mean that the most sophisticated model must be used to simulate the processes. Often, limitations in data, models, tools, and the conceptual site model will not support a more sophisticated model. In this case, the more sophisticated model may not provide an answer to a key question with any less uncertainty than a less sophisticated model. If it is determined that a more sophisticated model may reduce uncertainty by considering critical processes, then the cost of reducing this uncertainty must be considered.

Identify potential models or tools. Once the critical processes are identified, the modeler can begin to narrow down the list of potential models or tools to those that can address the critical processes within the specified limits on uncertainty and resources.

Identify modeling parameter data gaps. Data gaps may exist in the conceptual site model; however these data gaps can be addressed within the model by using standard default assumptions. Other parameters may need to be estimated on a site-specific basis. Once again, it is the question of “What is acceptable uncertainty?” that will determine what parameters must be assessed on a site-specific basis. A sensitivity analysis may assist in making these decisions. By identifying the impact of using a default value on the output of the model and

its associated uncertainty, the team can make an informed decision regarding the importance of a particular variable. For example, sensitivity analysis may show that good estimates of effective porosity may have a large impact on the estimated rate at which a contaminant moves but little impact on determining whether a contaminant will eventually migrate to a potential receptor. Depending on the key question that must be addressed, this particular parameter may be more or less important.

E.2.3.9 Provide the DQO team with potential modeling scenarios

The evaluation of available tools may result in the identification of a number of modeling options that could fulfill the modeling goals. Potential modeling scenarios are descriptions of the models that may be used, the critical processes that will be modeled with each model, and the site-specific modeling parameters that are currently data gaps. The purpose of these descriptions is to identify the uncertainties associated with applying any model. The modeling scenarios should answer the basic question "What does it mean if model A is selected instead of model B for transport of contaminants through a medium?". For each data gap, the value of collecting that piece of information should be discussed in terms of relative uncertainty reduction. At this point, the RI team may determine that no available modeling option can operate under the constraints identified in earlier steps. In this case, the decision is either to be satisfied with the level of uncertainty that will be created by not filling a data gap or to reexamine the constraints that have been placed on the project. For example, the project team, including the regulators, may decide to extend the schedule for several months while critical data are collected.

E.2.3.10 Determine data to be gathered

This step consists primarily of the final DQO meeting in this iteration of the process. The RI/FS team must weigh the modeling scenarios presented with the constraints on the project. The data to be collected must be decided upon based on the objectives that need to be fulfilled and weighed against the amount of uncertainty that can be accepted. For example, although taking 10 more soil samples would reduce the uncertainty involved in a risk assessment, the cost to the project would be great in terms of potential document delays and analytical costs. The project team must decide if the reduction in uncertainties would be worth the cost of resources. Most important at this step is the fact that modeling objectives are being considered as a part of DQOs development. If modeling is to play a role in risk assessment and remediation, its role must be well defined by applying the model selection and DQO processes in a complementary manner. In some cases this will result in the decision not to model in a particular situation. The decision not to model or not to gather data is just as important as the decision of what model or data to use for a particular situation.

E.2.3.11 Select model, gather data, and run model option

Selection of an appropriate model, or the decision not to model, is now apparent within the process. Once data collection is complete, and the model option is run, there must be a method to document the context within which results should be interpreted. Therefore, a sensitivity analysis and uncertainty analysis may be run as the final step in an iteration of the model selection process.

E.2.3.12 Conduct sensitivity analysis and uncertainty analysis

Sensitivity analyses are generally conducted to bracket the reasonable answers to the risk assessment or remedial action questions being posed. An evaluation of the uncertainty associated with the model predictions assists in the identification of the need for further study of the question at hand or a refined question. If the level

of uncertainty is acceptable, then the model predictions can be interpreted accordingly. However, if the resulting uncertainty is not acceptable, the sensitivity analysis will help to identify those parameters that, if measured on a site-specific basis, would decrease uncertainty to the greatest extent

Awareness of the environmental impact of releases of hazardous and radioactive wastes from storage facilities to the main sources of drinking water has grown dramatically. High priority efforts have been under taken to control and maintain releases at or below acceptable levels. Therefore, fate and transport modeling of potential releases of contamination to groundwater and surface water have become a main concern in the environmental arena. Evaluation of the fate and transport of contaminants is usually accomplished by employing the following four main diffusion-convection submodels:

- leaching contaminants from waste packages, trenches, and pits through the waste barrier;
- short range transport of contaminants from the burial site through the vadose zone to the saturated zone;
- transport of contaminants in the groundwater to potential receptors downgradient or to the surface water;
- transport of contaminants in the surface water to potential receptor downstream.

Several codes are available to simulate the release of contaminants from the different waste sites and transport through the unsaturated zone underneath (e.g., the DUST code). In addition, various codes are available to simulate the transport mechanism of the released contaminants to potential receptors (e.g., SESOIL, FTWORK, MEPAS). Although, these codes have been applied frequently at the Oak Ridge Reservation they do not provide an exhaustive list of the potential models which may be applicable at the Oak Ridge Reservation.

E.3. CONCLUSIONS

This brief guidance provides a paradigm for the application of a groundwater model selection process which should be followed when groundwater modeling is being considered in support of Environmental Restoration Program risk assessment activities. The single most important message to project managers and risk assessors is that the process of model selection must be started in the early phases of project scoping. It is the responsibility of the project manager to contact the program managers for risk assessment and geosciences to ensure that the appropriate personnel are involved so this process can be implemented in a timely manner. By considering the modeling needs of a project at the planning stages, the most appropriate model is used to meet project objectives, data needed to support modeling are identified, and the uncertainties associated with results are reduced.

It should not be assumed that groundwater transport modeling is needed for all risk activities. It is the intent of the Environmental Restoration Risk Assessment Program to limit the application of groundwater modeling to situations (1) where it is needed to support decisions and (2) when there is sufficient information to provide for meaningful results. In addition, if modeling is necessary, the complexity of the code should be the minimum level needed to meet the risk assessment and project objectives (e.g., if a “back-of-the-envelope” calculation is sufficient, a three-dimensional fracture flow computer code will not be used).

E.4 REFERENCES

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APPENDIX F

FOOD CHAIN MODELS FOR RISK ASSESSMENT

F.1 INTRODUCTION

Human health risks are generally modeled for a number of exposure scenarios following *Risk Assessment Guidance for Superfund: Volume 1-Human Health Evaluation Manua*l (RAGS) (EPA 1989a). Ingestion of contaminated foods is an important component of the agricultural scenario, yet detailed models addressing food ingestion exposures are not provided in RAGS. Humans may be exposed to site contaminants by eating vegetables or grains that have been contaminated through uptake of contaminants from soil and deposition of airborne contaminants on plant surfaces. Humans may also be exposed by eating meat or drinking milk produced by animals that have ingested contaminants in food, soil, water, or air. This document provides comprehensive models to be used in determining contaminant concentrations in foods eaten by humans. It provides default values for all parameters used in the models and explains how the models can be applied to risk assessment.

The Environmental Restoration (ER) Risk Assessment Program is providing these models to all organizations involved in risk assessment activities to ensure consistent development and application of food chain models in human health assessments for United States Department of Energy Oak Ridge Operations (DOE-ORO). Current recommendations for baseline human health risk assessments at Oak Ridge sites do not include the full agricultural scenario, but consideration of ingestion of homegrown produce is recommended under the future residential scenario (Miller et al. 1995). In addition, operable unit data should be screened against the agricultural preliminary remediation goals (PRGs) for beef and milk ingestion provided by DOE (1995).

The decision to fully evaluate food chain exposures must be determined on a site-by-site basis. Therefore, the ER Risk Assessment Program Manager should be consulted before incorporating food chain models into risk assessments to confirm the need for evaluation of food chain exposures. Parameters are provided for a number of exposure pathways that are not currently recommended for use at DOE-ORO (Miller et al. 1995); these values are provided for informational purposes and may be used if a particular pathway (i.e., ingestion of pork) is determined to be relevant at a site.

F.1.1 Applications

This report is meant to be a companion document to *Preliminary Remediation Goals for Use at the U.S. Department of Energy Oak Ridge Operation Office* (DOE 1995). However, the models developed here differ in several respects from the conservative screening models used in that report (DOE 1995). Where appropriate, models have been modified to incorporate more realistic exposure assumptions. Default values for some exposure parameters differ from those in the DOE report (1995) as a result of the extensive literature review conducted for this report. Specific differences are noted in the text associated with each model. The agricultural PRGs in the DOE report (1995) will be revised to incorporate new information obtained during development of this report.

The two primary models needed to determine contaminant concentrations in human foods are a plant model that accounts for uptake of contaminants from soil, water, and air and an animal model that accounts for transfer of contaminants ingested by animals to animal tissues eaten by humans. This report focuses on ingestion of beef, milk, leafy vegetables, and nonleafy vegetables. It does not include all possible human food sources. However, the models can be modified to address other food sources. Parameter values for some other food types (sheep, pork, chicken, eggs, goat, white-tailed deer) have been included where available for informational purposes; pathways involving these food types are not currently required or recommended for DOE-ORO assessments (Miller et al. 1995). The output from the models presented in this report provides an estimate of contaminant concentrations in plant and animal tissues that can be used as input into standard

models for determining chronic daily intakes for humans (i.e., those in DOE 1995). The models used in this report have been derived by examining models available in the open literature and combining or modifying them as necessary to account for all likely routes of exposure for plants and animals.

The general model for plants accounts for irrigation, aerial deposition, root uptake, and resuspension contributions to contaminant loads. If a given pathway is not expected to occur at a particular site, the model component accounting for that pathway can be set to zero. Results of the plant model (using parameter values for pasture) are used as input into the animal exposure models. Results of the plant model using leafy or nonleafy vegetable parameter values are used directly in human chronic daily contaminant intake models.

F.1.2 Model Development

The models provided in Sects. F.2 and F.3 were developed following an extensive review of available literature dealing with food chain modeling. Generally, two types of models were available: dynamic models and steady state models. Dynamic models separate components of the system into compartments (air, soil, water, plant, etc.) and describe the rate of change of contaminant levels into and out of the compartments using linear differential equations (NCRP 1984). Steady state models assume equilibrium among the various compartments. Relatively simple models are developed that include the primary parameters controlling uptake and transfer of contaminants. The decision was made to develop the simpler steady-state models for this report because they are readily applied, parameter values are more readily available, and data requirements are more similar to those available from standard remedial investigations.

Numerous terrestrial food chain models are available in the literature. Most of these models were developed to predict the transport of radionuclides through food chains, but the general procedures are also applicable to all nonvolatile contaminants. The models presented here do not apply to tritium or carbon-14 [see NCRP (1984, 1989) for discussion of models dealing with these special case radionuclides]. They focus on food chain exposures following release of radionuclides into the air; therefore, deposition is a primary concern. Models such as those developed by NRC (1977), Hoffman et al. (1982), IAEA (1982), NCRP (1984, 1989), Whelan et al. (1987) and EPA (1989b) differ slightly in the assumptions made regarding parameter values and in some of the specific parameters included to refine model outputs. While many models are available, the basic equations and principles underlying them are similar. The models provided in the following text build upon those commonly used in exposure assessments. Likely exposure routes have been added where appropriate [i.e., soil ingestion, a component left out of a number of the deposition-based models, has been included in the animal model because a number of studies have suggested that soil ingestion can be a significant exposure route (Thornton and Abrahams 1983)], and recent findings have been incorporated into models [i.e., the plant mass loading approach has been substituted for the resuspension factor approach to evaluate resuspension of contaminants from soil as recommended by Hinton (1992)].

F.1.3 Organization

Section F.2 of this report describes the general model recommended for estimating contaminant concentrations in plant parts eaten by animals and humans, assuming no irrigation. The primary exposure routes associated with contamination of plants (root uptake, aerial deposition, and resuspension from soil) are discussed individually, followed by a discussion of contamination resulting from irrigation of crops. Section F.3 of this report addresses the general and exposure route–specific models to be used in estimating contaminant concentrations in meat or milk products. Section F.4 describes the selection of default values for each parameter in the exposure models, including food type–specific values for select animals.

F.2 PLANT MODELS

For a complete analysis of food chain exposures for humans, it is necessary to estimate concentrations of contaminants in plants directly consumed by humans and in plants consumed by animals that are then eaten by humans. Plants may be exposed to contaminants as a result of direct deposition onto plant surfaces (wet and dry deposition, including resuspension), root uptake from soil, and irrigation with contaminated water. Resuspension accounts for contaminants deposited on soil that are resuspended in air by wind, rainsplash, or physical disturbance and subsequently deposited on plant surfaces. When possible, samples of plants or plant products should be used to estimate exposure concentrations (EPA 1989c). However, in the absence of measured plant concentrations, exposure models are appropriate for estimating these concentrations.

The general model for determining concentrations in plants can be applied both to crops eaten by humans and to plants that serve as animal foods, but the selection of parameter values varies depending on the type of plant considered and the management practices applicable to that plant type. The simplest models do not model wet and dry deposition or irrigation individually. Instead, they estimate plant concentrations by multiplying the measured soil concentration by a contaminant-specific biotransfer factor. This is the approach recommended in RAGS (Part A) (EPA 1989c) when soil is the source of contaminants. More detailed models attempt to account for wet and dry deposition rates and translocation of contaminants to edible plant tissues. If root uptake is the predominant exposure route for a particular chemical, the simple models are generally adequate. However, for contaminants that have very low soil-to-plant transfer factors or where deposition is continuous, resuspension and subsequent deposition can be the primary exposure routes. Therefore, the more detailed models are often necessary. RAGS suggests using air deposition modeling if deposition is the source of contaminants. The models recommended in this report include deposition and translocation in addition to root uptake from soil, but they may be modified to fit specific site conditions after consultation with the ER Risk Assessment Program Manager.

F.2.1 General Model

As noted previously, the general model for estimating contaminant concentrations in and on plants includes root uptake and foliar deposition from air and resuspended soil. Where irrigation is a significant management practice, components accounting for root uptake and resuspension of contaminants originating in irrigation water and direct deposition of irrigation water on plant surfaces can be added. Therefore, the comprehensive plant model for a site where irrigation is a consideration is:

$$C_{plant} = C_{plant-us} + C_{plant-da} + C_{plant-rs} + C_{plant-ui} + C_{plant-di} + C_{plant-ri} \quad , \qquad (1)$$

where

C_{plant} = concentration in and on plant estimated based on root uptake and foliar deposition (mg/kg or pCi/kg),
$C_{plant-us}$ = concentration in plant tissue resulting from root uptake from soil (mg/kg or pCi/kg),
$C_{plant-da}$ = concentration in edible parts of plant as a result of direct deposition of airborne contaminants (mg/kg or pCi/kg),
$C_{plant-rs}$ = concentration in edible parts of plant as a result of resuspension of contaminants associated with soil (mg/kg or pCi/kg),
$C_{plant-ui}$ = concentration in plant tissue associated with root uptake of contaminants resulting from irrigation

(mg/kg or pCi/kg),

$C_{plant\text{-}di}$ = concentration in edible parts of plant as a result of direct deposition of contaminants in irrigation water (mg/kg or pCi/kg),

$C_{plant\text{-}ri}$ = concentration in edible parts of plant as a result of resuspension of contaminants associated with irrigation water (mg/kg or pCi/kg).

The last three terms of this model are set to zero if irrigation is not a consideration. If airborne contamination is not a consideration, the direct deposition term may also be set to zero. Therefore, this model can be readily modified to fit a number of scenarios.

The following section provides detail on the estimation of each of the components in Eq. (1). The components used assuming no irrigation are discussed first, followed by the components associated with irrigation. Irrigation of pasture is not a common practice in east Tennessee (in the vicinity of the Oak Ridge Reservation), southern Ohio (in the vicinity of the Portsmouth Gaseous Diffusion Plant), or southwest Kentucky (in the vicinity of the Paducah Gaseous Diffusion Plant) because annual rainfall is generally adequate. Therefore, it is not necessary to include the irrigation components when estimating contaminant concentrations in pasture grasses consumed by livestock. However, vegetable crops usually are irrigated to some degree, so it is necessary to consider the irrigation components when estimating concentrations in vegetable crops. Recommended default values or appropriate literature sources for model parameters are provided in Table F.1.

F.2.1.1 Plant uptake without irrigation

F.2.1.1.1 Root uptake

Plants are exposed to contaminants in soil through root uptake. The model used to account for this exposure involves multiplying the soil concentration by a chemical-specific transfer coefficient. The transfer coefficients are defined as the ratio of the concentration of the chemical in plant tissue to the concentration in soil and are a measure of how much of the soil contamination is transferred to plant tissues. Site-specific transfer coefficients are most desirable, but in the absence of site-specific values, literature-based values for inorganic elements may be obtained from published reviews such as those by IAEA (1994), NCRP (1989), Ng et al. (1982) and Baes et al. (1984). The uptake of most heavy metals by edible plants usually occurs via their root systems (EPA 1989b). Transfer coefficients for organic chemicals can be obtained from chemical-specific studies or estimated using the relationship between transfer coefficients and chemical K_{ow}'s described by Travis and Arms (1988). Briggs et al. (1982, 1983) and Ryan et al. (1988) discuss plant uptake of non-ionic organic chemicals from soil (see Sect.F.4.1.1 for further discussion of transfer coefficients).

Table F.1. Recommended default values for parameters used in plant exposure models.

Parameter	Default	Range	Sources
BTF_{plant}, soil-to-plant transfer coefficient (kg dry soil/kg dry plant)	chemical and plant specific, see Sect.F.4.1.1	--	organic chemicals: Travis and Arms (1988), McKone (1994) inorganic chemicals: IAEA (1994), NCRP (1989), Baes et al. (1984)
d, deposition rate ($mg/m^2/d$)	calculated, see Sect.F.4.1.2	--	NCRP (1984)
V_d, deposition velocity (m/d)	1000	17-2333	Peterson (1983), NCRP (1989)

Table F.1. (continued)

Parameter	Default	Range	Sources
f_R, interception fraction (unitless):			
pasture			
leafy vegetables	0.42	0.02-0.82	Miller (1980)
nonleafy vegetables	0.42	0.06-1.2	Miller (1980)
spray irrigation	0.42	0.06-1.2	Miller (1980)
	0.25	0.23-0.38	NRC (1977), Miller (1980)
T, translocation factor (unitless)			
pasture			
leafy vegetables	1.0	--	NCRP (1984)
nonleafy vegetables	1.0	--	NCRP (1984)
	0.1	--	Baker et al. (1976), NCRP (1984)
Y, plant yield (kg/m^2)			
pasture (dry wgt.)			
Paducah	0.168	0.112-0.224	D. Wilson, pers. comm.
Portsmouth	0.112	--	J. Fisher, pers. comm.
general	0.33	0.04-1.59	Baes and Orton (1979)
leafy vegetables (wet wgt.)			
Paducah	2.0	--	NCRP (1984)
Portsmouth			
general	2.0	--	NCRP (1984)
nonleafy vegetables (wet wgt.)			
Paducah	0.62	0.112-1.12	D. Wilson, pers. comm.
Portsmouth			
general	2.0	--	NCRP (1984)
λ_E, removal constant -- plant (/d)	--	--	Estimated using weathering half-life (and radioactive decay constant for radionuclides)
t_w, weathering half-life (d)	14	2.8-34	NRC (1977), NCRP (1984, 1989), DOE (1995)
t_e, time of above-ground exposure (d)			
pasture			
produce	30	--	NRC (1977), NCRP (1984), Whelan et al. (1987)
	60	--	
MLF, mass loading factor (kg soil/ kg plant):			
pasture	0.25	<0.001-0.5	Hinton (1992)
leafy vegetables	0.26	--	Pinder and McLeod (1989)
nonleafy vegetables	0.11	0.008-0.21	Hinton (1992)
Ir, irrigation rate ($L/m^2/d$)			
pasture	0	--	
crops	3.62	--	DOE (1995)
Ip, irrigation period (unitless)	0.25	--	DOE (1995)
P, root zone soil density (kg/m^2)	240	170-267	Hoffman et al. (1982), Peterson (1983), McKone (1994)

Parameter	Default	Range	Sources
λ_B, removal constant -- soil (/d)	0.000027 + λ_i		Losses by means other than radioactive decay (NCRP, 1989) (+ radioactive decay constant for radionuclides)
λ_i, radioactive decay constant	0.693/half-life	--	see DOE (1995) for half-lives
t_b, buildup time (d)	10,950	--	NCRP (1984, 1989), DOE (1995)

The concentration of a contaminant in plant tissue as a result of root uptake from soil can be described as (EPA 1989c):

$$C_{plant-us} = C_{soil}\ BTF_{plant}\ , \qquad (2)$$

where:

$C_{plant-us}$ = concentration in plant tissue from root uptake from soil (mg/kg),
C_{soil} = concentration in upper 15 cm of soil (mg/kg) (measured),
BTF_{plant} = transfer factor from soil to plant tissue (mg/kg dry plant per mg/kg dry soil) (chemical- and species-specific, see Sect.F.4.1.1).

The soil concentration used as input into this model should be derived from measures of root zone soil. Depending on plant type and site conditions, plant rooting depths may vary from several centimeters to more than a meter. The bulk of roots that are actively engaged in the uptake of water and minerals occur in the upper 15–100 cm (Raven et al. 1981). Under plowed agricultural conditions, the root zone would nearly always be expected to be greater than 15 cm. The root zone in pasture could be less, but site-specific root zone measurements at DOE-ORO sites probably will not be performed. The default value recommended for root zone soil in this report is the upper 15 cm of soil. This corresponds to the depth used by the NRC (1977), Peterson (1983), and NCRP (1984).

The NCRP (1984) includes parameters to account for the chemical removal rate from soil in its equation for uptake by plants from soil. Whelan et al. (1987) do not include a component for removal rate from soil, nor is it included in RAGS (EPA 1989b). The removal rate from soil has not been included in the plant root uptake model presented here because this model is based on having measured or estimated soil concentrations available. If leaching or weathering from soil are expected to be significant factors at a site, these losses should be accounted for when determining soil concentrations to be input into the plant model [see NCRP (1984) for discussion of mechanisms for losses from soil].

SESOIL is an example of a model available for modeling soil concentrations over time (ORNL 1994). A constant meant to account for losses from soil is included in the root uptake and resuspension models under the irrigation scenario.

F.2.1.1.2 Aerial deposition

The aerial deposition component accounts for direct deposition of airborne contaminants onto plant surfaces. This component of the model is not necessary if the scenario being evaluated is restricted to soil or water sources rather than air. DOE (1995) assumed only soil and water sources; therefore, direct foliar deposition is not considered in its model. Deposition of contaminants resuspended from the soil surface and

subsequently deposited on plant surfaces is considered under resuspension and is relevant in these scenarios.

A general model for deposition of contaminants onto plant surfaces from air pathways is provided in Whelan et al. (1987) and NCRP (1984). The contaminant air-to-ground deposition rate is multiplied by the fraction of deposited material that is intercepted by plants and divided by the plant yield. The result is multiplied by a translocation factor to account for the fraction of deposited material that is transferred from external plant surfaces to the edible parts of the plant. This amount is then adjusted to account for losses due to weathering (and radioactive decay for radionuclides). The translocation factor is usually set at 1.0 for pasture and leafy vegetables and 0.1 for nonleafy vegetables (NCRP 1984).

$$C_{plant-da} = \frac{d\ f_R\ T}{Y} \frac{(1 - e^{(-\lambda_E\ t_e)})}{\lambda_E}\ , \qquad (3)$$

where:

$C_{plant-da}$ = concentration in edible parts of plant as a result of direct deposition of airborne contaminants (mg/kg),

d = deposition rate of contaminant from air to ground surface ($mg/m^2/d$). Calculated as the product of the air concentration (mg/m^3) and a chemical-specific average deposition velocity (m/d) (for default value, see Sect.F.4.1.2),

f_R = interception fraction. The fraction of deposited material intercepted and retained on foliage (unitless) (for default value, see Sect.F.4.1.3),

T = translocation factor. This factor accounts for translocation of externally deposited contaminants to edible parts of plants (unitless) (for default value, see Sect.F.4.1.4),

Y = standing plant biomass at harvest above a unit surface area or yield of crop (kg/m^2) (default value: site-specific, see Sect.F.4.1.5),

λ_E = the effective removal constant for given constituent from plant (per day). $\lambda_E = \lambda_i + 0.693/t_w$, where: t_w = weathering half-life, and λ_i = the radioactive decay constant for radionuclides [see NCRP (1989) Table 4]. λ_i is chemical-specific; t_w is 14 d (NRC 1977),

t_e = time of above-ground exposure of plant to contamination during the growing season (d) (site-specific, see Sect.F.4.1.7).

F.2.1.1.3 Resuspension

Contaminants in surface soil layers can be resuspended in air by wind or mechanical disturbances. Resuspended particles may then be deposited on plant surfaces. Contaminant concentrations are usually higher in soil than in plants, so even small amounts of soil on plant surfaces can make a significant contribution to ingestion exposures (Green and Dodd 1988, Pinder and McLeod 1988, Hinton 1992). For relatively insoluble elements, greater quantities may be ingested with soil particles on plant surfaces than those that have been incorporated into the internal tissues of the plant (Pinder et al. 1991). In environments where resuspension prevails, direct deposition on plant foliage may exceed root uptake (Adriano et al. 1980). Breshears et al. (1992) indicate that resuspension is crucial for predicting concentrations of ^{137}Cs in milk.

However, resuspension is not expected to be a major concern at DOE-ORO sites. Uncertainty associated with the resuspension route is significant (Corbett 1977). Resuspension factors and resuspension rates range over 7–8 orders of magnitude (Nicholson 1988). Humidity may reduce resuspension relative to that which takes

place in arid or semi-arid regions (Cohen 1977), possibly because humid regions generally have denser vegetation cover, and vegetation may reduce the likelihood of particles being resuspended. Many resuspension studies have been carried out in arid or semi-arid regions (Nicholson 1988). Over the long term, root uptake of contaminants is expected to exceed that from direct deposition at DOE-ORO sites.

Hinton (1992) provides a recent review of literature on contamination of plants by resuspension and critiques the methods used to estimate resuspension. Most of the current methods (i.e., resuspension factor approach, resuspension rate approach, air mass loading approach) were designed to examine inhalation rather than ingestion exposures. He concludes that "our understanding of the processes and mechanisms of resuspension onto plant surfaces are currently inadequate for accurate predictions." Parameters that potentially affect resuspension and soil adhesion to plants include characteristics of soil, contaminants, meteorological factors, agricultural factors, and plant characteristics (Hinton 1992). Hinton believes the plant mass loading approach has the most merit for understanding the processes of resuspension onto plants. The approach has been used by a number of researchers in agricultural systems of the southeastern United States over the last 10 years (Hinton 1992). Other approaches may be adequate if inhalation is the primary concern. Healy (1980) favored the air mass loading approach, but he did not review the plant mass loading approach.

The plant mass loading approach involves determining the mass of soil on vegetation per mass of dry vegetation. In the absence of directly measured plant concentrations, mass loading factors (MLF) can be multiplied by the concentration in the resuspendable soil fraction at the site to arrive at the plant concentration. The variation in plant mass loading factors is much less than that for resuspension factors (3 vs. 7 orders of magnitude) (Hinton 1992). The relative importance of surface soil contamination as compared to root uptake may be greater if contaminants are concentrated in small-sized soil particles or have been recently deposited on the soil surface (Pinder et al. 1991). Pinder and McLeod (1988) note that the difference between concentrations in suspendable materials and that in the upper 50 mm of soil may result in underestimates of plant mass loading. Where possible, measures of contaminant concentrations in the resuspendable portion of soil should be used in developing plant mass loading factors. In practice, measures of resuspendable soils are unlikely to be conducted as part of the remedial investigation process, and the default MLF provided in Table F.1 should be used.

Using the plant mass loading approach, the contribution of resuspension from soil to the plant contaminant load can be estimated as the product of the measured soil concentration and the plant mass loading factor (Hinton 1992):

$$C_{plant-rs} = MLF \; C_{soil} \; , \qquad (4)$$

where:

$C_{plant-rs}$ = concentration in edible parts of plant as a result of direct deposition of airborne contaminants resulting from resuspension from soil (mg/kg),
C_{soil} = concentration of the contaminant measured in resuspendable soil fraction (mg/kg) (default value: measured),
MLF = mass-loading factor (kg soil/kg dry plant) (default value: site-specific, see Sect. F.4.1.8).

Use of a soil concentration based on soil components other than the resuspendable fraction, such as total surface soil concentration, will result in likely underestimation of actual concentrations resulting from resuspension. The upper 15-cm of soil is commonly used, but even this includes soil deeper than is likely to be resuspended. Where plowing agricultural land has resulted in thorough mixing of soils, this should not be

a major concern.

F.2.1.2 Plant uptake with irrigation

Plants may be irrigated with surface water or groundwater using spray or flood irrigation practices. Root uptake and resuspension are relevant under both spray and flood irrigation, but aerial deposition is only relevant for spray irrigation. The models for plant uptake resulting from irrigation are similar to those without irrigation except for the use of water concentrations in place of soil or air concentrations and incorporation of the irrigation rate and irrigation period.

F.2.1.2.1 Root uptake from irrigation

The following equation for determining contaminant uptake by plant roots as a result of irrigation was modified from Whelan et al. (1987), NCRP (1984), and DOE (1995):

$$C_{plant-ui} = \frac{C_{water}\ Ir\ Ip\ BTF_{plant}}{P}\frac{(1 - e^{(-\lambda_B\ t_b)})}{\lambda_B} \quad , \qquad (5)$$

where:

$C_{plant-ui}$ = concentration in plant tissue from root uptake due to irrigation (mg/kg),
C_{water} = concentration in water used for irrigation (mg/L) (default value: measured),
Ir = irrigation rate ($L/m^2/d$) (default value: site-specific, see Sect.F.4.1.9),
Ip = irrigation period = fraction of year plants are irrigated (unitless) (default value: site-specific, see Sect.F.4.1.9),
BTF_{plant} = transfer factor from soil to plant tissue (mg/kg dry plant per mg/kg dry soil) (default value: chemical- and species-specific, see Sect.F.4.1.2),
P = root zone soil density (kg/m^2) (default value: site-specific, see Sect.F.4.1.10),
λB = the effective removal constant for given constituent from soil (per day) [default value: λ_i + 0.000027 (NCRP 1989)],
t_b = long-term deposition and buildup (d) (default value: site-specific, see Sect.F.4.1.12).

F.2.1.2.2 Aerial deposition from irrigation

The concentration of a contaminant in plant tissue as a result of irrigation water deposited on the plant surface is similar to that for direct deposition from air. However, the deposition rate is the product of the concentration in the irrigation water and the irrigation rate rather than the air concentration times the deposition velocity:

$$C_{plant-di} = \frac{C_{water}\ Ir\ Ip\ f_R\ T}{Y}\frac{(1 - e^{(-\lambda_E\ t_e)})}{\lambda_E} \quad , \qquad (6)$$

where:

$C_{plant-di}$ = concentration in edible parts of plant as a result of direct deposition of contaminants in irrigation water (mg/kg)

C_{water} = concentration of contaminant in irrigation water (mg/L) (default value: measured),
Ir = irrigation rate (L/m^2-d) (default value: site-specific, see Sect.F.4.1.9),
Ip = irrigation period (unitless); fraction of year crops are irrigated (default value: site-specific, see Sect.F.4.1.9),
f_R = interception fraction; the fraction of deposited material intercepted and retained on foliage (unitless) (default value: spray irrigation–specific, see Sect.F.4.1.3),
T = translocation factor; this factor accounts for translocation of externally deposited contaminants to edible parts of plants (unitless) (for default value, see Sect.F.4.1.4),
Y = standing plant biomass at harvest above a unit surface area or yield of crop (kg/m^2) (default value: site-specific, see Sect.F.4.1.5),
λ_E = the effective removal constant for given constituent from plant (per day). $\lambda_E = \lambda_i + 0.693/t_w$, where t_w = weathering half-life -- the time required for half of the originally deposited material to be lost from the plant, and λ_i = the radioactive decay constant for radionuclides [default values: λ_i is chemical-specific; t_w is 14 d (NRC 1977)],
t_e = time of above-ground exposure of plant to contamination during the growing season (d) (Whelan et al. define as growing period of crop) (default value: site-specific, see Sect.F.4.1.7).

.2.1.2.3 Resuspension from irrigation

A resuspension component exists for the irrigation scenario which incorporates the irrigation rate and decay and leaching loss rate into the model for resuspension from soil. Essentially, the concentration in soil resulting from irrigation is used as input into the model for resuspension from soil.

$$C_{plant-ri} = MLF\ C_{water}\ \frac{Ir\ Ip}{P}\frac{(1 - e^{(-\lambda_B\ t_b)})}{\lambda_B}\ , \qquad (7)$$

where:

$C_{plant-ri}$ = concentration in edible parts of plant as a result of direct deposition of airborne contaminants resulting from resuspension from irrigation (mg/kg),
MLF = mass-loading factor (kg soil/kg dry plant) (default value: site- and plant type–specific, see Sect.F.4.1.8),
C_{water} = concentration of contaminant in irrigation water (mg/L) (default value: measured),
Ir = irrigation rate (L/m^2-d) (default value: site-specific, see Sect.F.4.1.9),
Ip = irrigation period = fraction of year plants are irrigated (unitless) (default value: site-specific, see Sect.F.4.1.9),
P = root zone soil density (kg/m^2) (default value: site-specific, see Sect.F.4.1.10),
λ_B = the effective removal constant for given constituent from soil (per day) [default value: λ_i + 0.000027 (NCRP 1989)],
t_b = long-term deposition and buildup (d) (Note: Whelan et al. use te_p which is defined as the duration of the growing period for the crop. NCRP 1984 uses t_b) (default value: site-specific, see Sect.F.4.1.12).

F.3 ANIMAL MODELS

F.3.1 General Model

Animals may be exposed to contaminants through ingestion of contaminated food, soil, and water, inhalation of contaminants suspended in air, and absorption of contaminants through their skin. Humans may be exposed to contaminants in animal tissues they consume. EPA's RAGS (1989a) recommends use of tissue monitoring data when available and appropriate for estimating human exposure to chemicals in the terrestrial food chain. In the absence of tissue data, EPA recommends the use of biotransfer factors (BTFs) and ingestion rates for estimation of animal tissue concentrations (EPA 1989c). This report presents a general model for estimation of the concentration of contaminants in the tissues of animals commonly eaten by humans. The concentrations estimated using this model can be input directly into human exposure models.

The model discussed in the following text is derived from models presented in NRC (1977), Peterson (1983), NCRP (1984, 1989), Whelan et al. (1987), and DOE (1995), among others. Many different models are available but nearly all follow the same general format. While both dynamic and equilibrium models exist in the literature, equilibrium models are used here because they are straight-forward, and values are generally available for parameters in the model. This white paper deals exclusively with ingestion exposures. Therefore, potential inhalation and dermal exposures for birds and mammals are not considered. While these routes of exposure are generally not significant for terrestrial vertebrates relative to ingestion pathways (NRC 1977), there may be scenarios in which they are more important. The ER Risk Assessment Program Manager should be consulted to determine whether inhalation or dermal contact should be addressed. The animal model is of essentially the same form for all species considered. Use of species-specific ingestion rates and biotransfer factors (when available) account for differences between species. The basic components are exposure through ingestion of food, soil, and water:

$$C_{animal} = C_{animal-food} + C_{animal-soil} + C_{animal-water}\ , \qquad (8)$$

where:

C_{animal} = concentration of contaminant in animal muscle (mg/kg),
$C_{animal\text{-}food}$ = concentration of contaminant in animal muscle obtained from ingestion of contaminated food (mg/kg),
$C_{animal\text{-}soil}$ = concentration of contaminant in animal muscle obtained from ingestion of contaminated soil (mg/kg),
$C_{animal\text{-}water}$ = concentration of contaminant in animal muscle obtained from ingestion of contaminated water (mg/kg).

Food, soil, and water concentrations are multiplied by their respective ingestion rates and by a contaminant-specific biotransfer factor (food-to-tissue), then summed to obtain the concentration of individual contaminants in tissue (EPA 1989b). For herbivorous animals, the results of the plant model are used as input for food concentration. Food-to-animal tissue BTFs are generally the only BTFs available. When they are unavailable for soil-to-tissue and water-to-tissue, it is assumed that contaminant transfer from soil- and water-to-tissue is similar to that for food-to-tissue. Therefore, the same BTF is used for each exposure route. RAGS cites Ng et al. (1977, 1979, and 1982) and Baes et al. (1984) as sources of BTFs for food-to-beef and food-to-milk. However, more recent sources include NCRP (1989) and IAEA (1994). These are recommended as the primary sources of metal uptake values. Muscle is the tissue most frequently eaten by humans, and BTFs are

generally available for transfer from food to muscle. BTFs for other tissues are more limited in availability. However, the general model discussed here can be used to determine concentrations in other tissues (i.e., liver).

The general model is made more realistic by including terms to account for the portion of the year the animals ingest food from the site (time on pasture for beef and dairy cattle), the proportion of the animal's diet which comprises food from the site while the animal is on the site (percent pasture in diet while on pasture), and the proportion of the site which is actually contaminated (for cattle grazing pasture, if only 50% of pasture is contaminated, this can be accounted for in the model). Site-specific values for these management related parameters should be obtained from local agricultural extension agents. Recommended default values for exposure parameters are provided in Table F.2.

Table F.2. Recommended default values for parameters used in animal exposure models

Parameter	Default	Range	Sources
BTF_{animal}, wet weight transfer coefficient from daily intake to edible portion of animal product (pCi or mg/kg (or L) meat, eggs, or milk over pCi or mg/d)	chemical-, animal-, and tissue- specific, see Sect.F.4.2.1	--	Organic chemicals: Travis and Arms (1988), McKone (1994) Inorganic chemicals: IAEA (1994), NCRP (1989), Baes et al. (1984)
IR_{food}, daily food ingestion rate (kg/d on dry weight basis)			IAEA (1994)
beef cattle (500 kg)	7.2	5–10	
dairy cattle	16.1	10–25	
sheep	1.3	1–2.5	
goats	1.3	1–3.5	
swine (110 kg)	2.4	2–3	
chickens	0.07	0.05–0.15	
laying hens	0.1	0.07–0.15	
f_p, fraction of the year the animal is on the site (unitless)			
Paducah:			
beef cattle	1.0	--	McCracken Co. Extension Center, personal communication (1995)
dairy cattle	1.0	--	
sheep	1.0	--	
swine	0	--	
chickens	0	--	
Portsmouth:			
beef cattle	0.75	--	Ohio State University Extension Office, personal communication (1995)
dairy cattle	0.75	--	
sheep	0.75	--	
swine	0.67	--	
General:			
beef cattle	1.0	--	
dairy cattle	1.0	--	
sheep	1.0	--	
swine	0	--	
chickens	0	--	
f_s, fraction of the animal's food that is from the site (unitless)			
Oak Ridge:			
beef cattle	.90	.85–.90	Roane Co. Extension Agent, personal communication (1995)
dairy cattle	.60	--	
Paducah:			
beef cattle	.95	--	McCracken Co. Extension Center, personal communication (1995)
dairy cattle	.30	--	
Portsmouth:			
beef cattle	1.0	--	Ohio State University Extension Office, personal communication (1995)
dairy cattle	.60	--	
f_w, fraction of water obtained from site (unitless)	1.0	--	Whelan et al. (1987)

Table F.2. (continued)

Parameter	Default	Range	Sources
IR_{water}, daily water ingestion rate (L/d)			
beef cattle: general			
Paducah	50	--	IAEA (1994)
	37.8	--	McCracken Co. Extension Center,
dairy cattle: general			personal communication (1995)
Paducah	75	--	NRC (1981), IAEA (1994)
	56.8	--	McCracken Co. Extension Center,
sheep			personal communication (1995)
goats	6	--	NAS (1972), IAEA (1994)
	8	--	Bond and Straub (1975), IAEA (1994)
swine			NAS (1972), IAEA (1994)
chickens	8	--	NAS (1972)
white-tailed deer	0.2	--	Lautier et al. (1988)
	3.61	--	
IR_{soil}, daily soil ingestion rate for animals (kg/d)			
beef cattle	1.0	--	IAEA (1994)
dairy cattle	1.0	--	IAEA (1994)
sheep	0.13	--	IAEA (1994)
goats	0.03	--	judgement based on deer
swine	0.10	--	McMurter et al. (1993)
chickens	0.0014	--	NRC (1984), McKone (1994)
white-tailed deer	0.005	--	Beyer et al. (1994)
f_a, fraction of area that is contaminated (unitless)	1.0	--	conservative assumption, should use site-specific value

F.3.1.1 Food ingestion

The contaminant concentration in animal tissue resulting from ingestion of contaminated food is estimated by multiplying the biotransfer factor from food to tissue by food contaminant concentration, food ingestion rate, time on site, and percent food obtained from the site:

$$C_{animal-food} = BTF_{food-tissue}\ C_{food}\ IR_{food}\ f_p\ f_s\ , \qquad (9)$$

where:

$C_{animal-food}$ = concentration in animal tissue resulting from ingestion of contaminated food (mg/kg),

$BTF_{food-tissue}$ = biotransfer factor (d/kg on wet weight basis); calculated as the concentration of contaminant in animal tissue (mg/kg) divided by the contaminant intake rate (mg/d) (default value: chemical- and species-specific, see Sect.F.4.2.1),

C_{food} = concentration of contaminant in food eaten by the animal (mg/kg on *dry weight basis*); this is measured directly or modeled using equation presented in the plant model section (default value: measured or estimated using plant models),

IR_{food} = daily food ingestion rate for the animal (kg/d on *dry weight basis*) [Note: IR and C_{food} need to be on the same basis (wet or dry). The BTF should be wet weight because desired result is wet weight tissue concentration for input into human health exposure models.] (default value: site- and species-specific, see Sect.F.4.2.2),

f_p = faction of the year the animal is on the site (unitless); ts is the time on pasture for most livestock (default value: site- and species-specific, see Sect.F.4.2.3),

f_s = fraction of the animal's food that is from the site (unitless); this is the fraction of the diet that is pasture while on pasture for most livestock and accounts for the common practice of supplemental feeding while animals are on pasture (default value: site- and species-specific, see Sect.F.4.2.4).

F.3.1.2 Soil ingestion

Contaminant concentrations in animal tissue resulting from the ingestion of soil, deliberately or incidentally while feeding or grooming, is estimated by multiplying the soil ingestion rate by the ingestion-to-tissue transfer coefficient, the soil concentration, time on site, and fraction of the site that is contaminated:

$$C_{animal-soil} = BTF_{soil-tissue}\ C_{soil}\ IR_{soil}\ f_p\ f_a\ , \qquad (10)$$

where:

$C_{animal-soil}$ = concentration of contaminant in animal tissue as a result of soil ingestion (mg/kg),

$BTF_{soil-tissue}$ = biotransfer factor (d/kg on wet weight basis). Calculated as the concentration of contaminant in animal tissue (mg/kg) divided by the contaminant intake rate (mg/d). Because soil-to-tissue values are largely unavailable, food-to-tissue BTFs are used. (default value: chemical- and species-specific, see Sect.F.4.2.1),

C_{soil} = concentration of contaminant in soil eaten by the animal (mg/kg on dry weight basis) (default value: measured or modeled),

IR_{soil} = daily soil ingestion rate for the animal (kg/d on dry weight basis) (default value: site- and species-specific, see Sect.F.4.2.5)

f_p = fraction of the year the animal is on the site (unitless); this is the time on pasture for most livestock (assume animal ingests uncontaminated soil when it is off-site (default value: site- and species-specific, see Sect.F.4.2.3),

f_a = fraction of the site that is contaminated (unitless); if only half the site is affected by contamination, presumably only half of the soil ingested would contain contaminants (default value: site-specific, see Sect.F.4.2.6).

F.3.1.3 Water ingestion

Contaminant concentrations in animal tissue resulting from ingestion of contaminated water, while generally minor relative to those from food and soil ingestion, are estimated by:

$$C_{animal-water} = BTF_{water-tissue}\ C_{water}\ IR_{water}\ f_w\ , \qquad (11)$$

where:

$C_{animal-water}$ = concentration in animal tissue resulting from ingestion of contaminated water (mg/kg),

$BTF_{water-tissue}$ = biotransfer factor (d/kg on wet weight basis). Calculated as the concentration of contaminant in animal tissue (mg/kg) divided by the contaminant intake rate (mg/d). Because water-to-tissue values are largely unavailable, food-to-tissue BTFs are used.(default value: chemical and species-specific, see Sect.F.4.2.1),

C_{water} = concentration of contaminant in water consumed by the animal (mg/L) (default value: measured or modeled),

IR_{water} = daily water ingestion rate for the animal (L/d) (default value: site- and species-specific, see Sect.F.4.2.7),

f_w = fraction of daily water consumption that is contaminated (unitless); this is the fraction of daily water intake from the site (default value: site specific, see Sect. F.4.2.8).

F.3.1.4 Modifications to general model

The general animal model applies to the estimation of concentrations in milk with few adjustments. Biotransfer factors for transfer of contaminants from ingestion to milk should be used in place of those for transfer from ingestion to muscle. In addition, values for food, water, and soil ingestion rates specific to dairy cattle should be used. Dairy cows generally have higher energy requirements to support milk production; therefore, when eating similar feeds, their intake rates are higher than those for beef cattle.

The general model applies to bird and animal species expected to be exposed to contaminants at the site. Species-specific BTFs and food, water, and soil ingestion rates must be used as inputs into the model. As for milk, the general model can be used to estimate concentrations in eggs. Parameter values for chickens are used along with BTFs specific to transfer of contaminants from food to eggs.

If other sources of food, soil, or water are believed to contain contaminants, terms may be added to the general model. For instance, cattle fed stored feed may be exposed to contaminants in the feed. Therefore, a component that accounts for the fraction of the cattle diet composed of stored feed can be added.

F.4 DISCUSSION OF PARAMETER VALUES

Suggested default values for exposure parameters are provided in Tables F.1 and F.2. This section further discusses selection of those values.

F.4.1 Plant Models

F.4.1.1 Soil-to-plant transfer coefficients, BTF_{plant}

Transfer coefficients reported in the literature can vary widely because of the effects of different soil and vegetation types and environmental conditions involved in their estimation (IAEA 1994). Management practices such as plowing, liming, fertilizing, and irrigating can also affect uptake. Therefore, site-specific values are preferred over literature values that may have been derived under conditions dissimilar to those at the site under investigation.

However, in the absence of site-specific values, soil-to-plant transfer coefficients for many inorganic elements are available from reviews such as those by IAEA (1994), NCRP (1989), Baes et al. (1984), and Ng et al. (1982). The IAEA (1994) values should be used preferentially. Most of these values were derived as part of a large International Union of Radioecologists project in which research techniques were standardized to minimize artifacts and misinterpretations (IAEA 1994). Values have been standardized for a homogeneously contaminated soil layer of 20 cm for crops and 10 cm for pasture. Values have also been adjusted to standardized pH values: 6 for clay, 5 for sand, and 4 for peat soils. Higher pH values result in decreased uptake. For plants consumed by humans, the transfer factors refer to the edible parts of the plant. For plants eaten by animals, the transfer coefficients generally refer to the whole plant. IAEA (1994) provides species-specific transfer factors for many elements. Risk assessors should select values for the plant types that most

closely match the plant types of interest in the assessment area. Values presented in the IAEA (1994) report are on a dry-weight plant basis. Values for inorganic elements missing from the IAEA report should be obtained from NCRP (1989), Baes et al. (1984), or a specific study addressing uptake of the element by plants.

Soil-to-plant transfer coefficients for organic chemicals are less widely available. Where possible, actual measured values should be used. In the absence of measured data, uptake of contaminants into above-ground plant parts can be estimated using the relationship between the octanol-water partition coefficient of the chemical and uptake (Travis and Arms 1988) as modified by McKone (1994):

$$BTF_{plant} = 7.7\ K_{ow}^{-0.58}\ , \qquad (12)$$

where:

BTF_{plant} = measure of uptake into above-ground vegetation expressed as mg contaminant/kg above-ground plant (fresh weight) over mg contaminant/kg root zone soil (dry weight),
K_{ow} = octanol-water partitioning coefficient for the organic chemical.

This equation can be used directly for vegetable crops to be consumed by humans. For pasture crops that will be ingested by animals, it is more convenient to obtain the transfer factor on a dry-weight basis because plant intake rates for livestock are generally presented on a dry-weight basis rather than on a wet-weight basis. Therefore, the equation provided in Travis and Arms (1988):

$$BTF_{plant} = 38\ K_{ow}^{-0.58}\ , \qquad (13)$$

can be used directly for uptake into the above-ground parts of pasture plants.

For uptake by edible root crops, McKone (1994) modified the original Travis and Arms (1988) equation to incorporate information on uptake into plant roots described in other studies:

$$BTF_{plant} = 270\ K_{ow}^{-0.58}\ , \qquad (14)$$

where

BTF_{plant} = measure of uptake into plant roots expressed as mg contaminant/kg plant roots (fresh weight) over mg contaminant/kg root zone soil (dry weight),
K_{ow} = octanol-water partitioning coefficient for the organic chemical.

Octanol-water partitioning coefficients for organic chemicals are available from MEPAS (Strenge and Peterson 1989). Other sources include Lyman et al. (1982), Verschueren (1983), Howard (1989), and Mackay et al. (1992).

F.4.1.2 Deposition rate, d, and deposition velocity, V_d

The deposition rate (d) is a measure of the mass of material deposited from air to a unit area of ground per day. It can be obtained by multiplying the air concentration (pCi or mg/m^3) by the deposition velocity (m/d) (NCRP 1984). The air concentration can be measured at the height of the vegetation or at a reference height

(i.e., 1 m), or it can be determined using the air mass loading approach recommended by Healy (1980). Using the air mass loading approach, the air concentration of the contaminant is the product of the soil contaminant concentration and the concentration of soil particles in the air. A reasonable default value for the concentration of soil particles in air is 100 ug/m^3 (EPA 1977, Healy 1980). Deposition velocity relates the concentration above the surface to the deposition to the surface. The suggested default deposition velocity is 1000 m/d (NCRP 1989). This value includes both wet and dry deposition and is near the middle of the range (17–2333 m/d) reported for iodine by Peterson (1983). Therefore, the default deposition rate (mg/m^2-d) is the product of the air mass loading factor (0.0001 kg/m^3), the measured or modeled soil contaminant concentration (mg/kg), and the deposition velocity (1000 m/d).

F.4.1.3 Interception fraction, f_R

The interception fraction accounts for the proportion of aerial deposition that is intercepted by plant surfaces. The interception fraction varies with plant type and density of vegetation. NRC (1977) and NCRP (1984) use a default value of 0.25 for pasture grasses and 0.2 for vegetable crops. NCRP (1989) used 0.25 as the default for both vegetables and pasture. However, Miller (1980) reviewed a number of studies and reported a range of 0.02–0.82 for various grasses. The midpoint of this range (0.42) is suggested as the default value for use in the pasture plant models in this report. Interception fractions for vegetable crops ranged from 0.06–1.2 (Miller 1980), but 10 of 13 values were less than 0.49. The value of 0.42 used for pasture grasses is also suggested as the default for vegetable crops. Breshears et al. (1992) examined a number of values and determined that the geometric mean for the interception fraction was 0.39. The reader should note that there is considerable variability in the interception fraction values. Iodines exhibit a greater tendency to be retained on vegetation. The default iodine value of 1.0 from NRC (1977) is recommended in this white paper for both pasture and vegetable crops. The recommended value for interception of particles deposited by spray irrigation is 0.25; this is the default value used by NRC (1977) and is within the range reported by Miller (1980).

F.4.1.4 Translocation factor, T

The translocation factor is used to account for movement of contaminants from plant surfaces on which they were deposited to the edible portions of plants. The edible portion of leafy vegetables and pasture grasses are the leaf surfaces, so the translocation factor is set to 1.0 for these plant types (NCRP 1984). Translocation from leaf surfaces to the edible portion of nonleafy vegetables, fruits, and grains is a consideration, but data to support translocation values are limited. IAEA (1994) provides values for translocation of 16 elements in grains. While the values range from 0.0004 to 0.3, nearly all were less than 0.1. Hinton (1994) discusses translocation of cesium, strontium, and iodine in winter barley and wheat, root vegetables, other vegetables, and fruits. With the exception of potatoes (0.5), all values were $\leq$0.02. Therefore, the default value of 0.1 used by NCRP (1984) for nonleafy vegetables appears to be adequate and is suggested for use here as well.

F.4.1.5 Plant yield, Y

Plant yield is used in deposition models to account for the mass per unit surface area upon which particles are deposited. Data on yields of various plant types should be readily available on a site-specific basis. The yield of pasture grasses in the Portsmouth, Ohio, area is 0.448 kg (wet weight)/m^2 (personal communication, J. Fisher, Ohio State University Extension Service, 1995). Assuming pasture grasses are 75% water, this translates to a dry weight yield of 0.112 kg/m^2. The wet weight yields of pasture grasses, nonleafy vegetables, root vegetables, and fruits in the Paducah, Kentucky, area are 0.448–0.896, 0.112–1.12, 0.224–1.12, and 0.112–1.12, respectively (personal communication, D. Wilson, McCracken County Extension Center, 1995). The dry weight pasture yields are 0.112–0.224; the midpoint of 0.168 kg/m^2 is selected as the default value for pasture yield in the Paducah region. It is unnecessary to convert yields for crops destined for human

consumption to a dry-weight basis because human plant intake rates are generally given as wet weights. The default values suggested for nonleafy vegetables, root vegetables, and fruits (0.62, 0.67, and 0.62, respectively) represent the midpoints of the ranges provided by the county agriculture extension office. If site-specific data are unavailable, a default value of 2.0 kg (wet weight)/m^2 can be used for leafy and nonleafy vegetables (NCRP 1989). Yield of pasture grasses ranged from 0.04–1.59 kg dry plants/m^2 in the 257 studies examined by Baes and Orton (1979). The median value of 0.33 kg dry/m^2 (Baes and Orton 1979) is recommended as the default value for pasture grasses.

F.4.1.6 Weathering and decay constant, λ_E

The weathering and decay constant accounts for removal of deposited material from plant surfaces as a result of weathering processes and, for radionuclides, radioactive decay. The constant is estimated by adding the radioactive decay constant for radionuclides, λ_i, to the quotient 0.693 divided by the weathering half-life, t_w. The weathering half-life is the time required for half of the originally deposited material to be lost from the plant (NCRP 1984). The default weathering half-life of 14 days used by NRC (1977), NCRP (1984, 1989), and DOE (1995) is selected as the default in this report.

F.4.1.7 Above-ground exposure time, t_e

This parameter is defined as the time of above-ground exposure of a crop to contamination during the growing season (NCRP 1984). While it varies with plant type and with the growing season for a particular region (Hoffman et al. 1982), standard practice has been to use 30 days for pasture grasses and 60 days for produce (NRC 1977, NCRP 1984, Whelan et al. 1987, DOE 1995). Thirty days for pasture grasses is meant to represent animal grazing habits (Whelan et al. 1987), and 60 days represents the approximate growing time for vegetable crops.

F.4.1.8 Plant mass loading factor, MLF

The plant mass loading factor is defined as the ratio of the mass of soil on vegetation per mass of dry vegetation (Hinton 1992). It is multiplied by the contaminant concentration in resuspendable soil to determine the concentration of the contaminant deposited on the plant via resuspension. While it would be better to have site-specific mass loading factors, those from published studies can be used when site-specific values are unavailable. Hinton (1992) provides a compilation of much of the literature on plant mass loadings.

Values for a number of vegetation types and geographic areas range over 2–3 orders of magnitude. While mass loading factors are usually presented in mg soil/g dry plant, the values used here have been converted to kg soil/kg dry plant for direct input into the model. Mean plant mass loadings for pasture range from <0.001 to 0.5 kg soil/kg plant (Hinton 1992). Much of the variation may be due to differences in estimation and sampling methods. The default plant mass loading selected for pasture is 0.25 kg soil/kg plant. Pinder and McLeod (1989) report a mean plant mass loading on lettuce in South Carolina of 0.26 $\pm$0.10. The value of 0.26 kg soil/kg plant is selected as the default for leafy vegetables. Plant mass loading factors are higher for broadleaf crops whose leaves grow close to the ground surface (Pinder and McLeod 1988). Values for nonleafy vegetables range from 0.008 for soybeans to 0.21 for squash (Hinton 1992). The suggested default for nonleafy vegetables is the approximate midpoint of this range, 0.11 kg soil/kg plant.

F.4.1.9 Irrigation rate, Ir, and irrigation period, Ip

The irrigation rate and irrigation period define the amount and duration of water applied to crops. Irrigation of pasture is not a common practice in eastern Tennessee, southern Ohio, and southwestern Kentucky

because average rainfall amounts in these areas are adequate for pasture growth. However, irrigation of crops is a common practice. Ideally, site-specific data on irrigation rates should be used. DOE (1995) reports a value of 3.62 L/m^2-d obtained from the Roane County, Tennessee, extension agent; this is the default irrigation rate value. A default irrigation period of 0.25 is selected assuming crops will be irrigated three months out of the year. These defaults correspond to irrigation rates of approximately 32.5 cm (12.8 in.) per growing season.

F.4.1.10 Root zone soil density, P

While plant rooting depths vary depending on species and soil conditions, a typical depth used in a number of exposure models is 15 cm (NRC 1977, NCRP 1984, Peterson 1983). This is considered a typical depth for the plow layer. Soil density (kg/m^3) is multiplied by the rooting depth to obtain the root zone soil density, or areal soil density, in kg dry soil/m^2. McKone (1994) and Peterson (1983) use 1600 kg/m^3 as a typical soil density. Multiplying 1600 kg/m^3 by the typical plow layer depth of 0.15 m results in a root zone soil density of 240 kg/m^2; this is the recommended default value, which is well within the 95% percentile range of 170–267 reported by Hoffman et al. (1982) and is the same as that used by NRC (1977) and NCRP (1984).

F.4.1.11 Removal constant from soil, λ_B

The rate of contaminant removal from soil is usually equated with the radioactive decay constant (Baker et al. 1976, NRC 1977). However, if contaminant build-up time is estimated over thousands of years, other loss mechanisms (harvesting, leaching) should also be included (NCRP 1984). DOE (1995) estimates λ_B as the sum of the radioactive decay constant (0.693/radioactive half-life) and the rate constant for losses due to harvesting and leaching. NCRP (1989) uses a 70-year removal half-time of 0.000027/d for harvesting and leaching; this is near the geometric mean (0.000067) and within the 95% range (0.0000012–0.0037) for losses from soil by means other than radioactive decay reported by Hoffman et al. (1984).

F.4.1.12 Long-term deposition and buildup, t_b

The time for buildup of contaminants in soil depends on the duration of deposition; this should be determined on a site-specific basis. The default value (10,950 days) used by DOE (1995) and NCRP (1984, 1989) is based on a 30-year build-up time. The normal operating lifetime for a nuclear facility is 30–40 years. NRC (1977) used 5475 days assuming a build-up time of 15 years. The default suggested here is 10,950 days, but site-specific values are preferred.

F.4.2 Animal Models

F.4.2.1 Biotransfer factor, $BTF_{food\text{-}tissue}$

The ratio of contaminant concentration in animal tissue (mg contaminant/kg tissue, wet weight) to daily intake (mg contaminant/d) is defined as the biotransfer factor. It is a measure of how much of what an animal ingests is actually transferred to tissue. For estimation of human exposures, muscle is the tissue of interest. The BTF (d/kg) is multiplied by a species-specific food ingestion rate (kg/d) and by contaminant concentration in food (mg/kg) to obtain an estimate of the concentration in meat in mg contaminant/kg meat. BTFs are both chemical- and species-specific. In addition, they are influenced by site conditions, so site-specific values are preferred, when available.

BTFs are unavailable for many livestock species and are limited for tissues other than muscle. EPA (1993a) proposed normalizing available transfer factors based on lipid content of the organisms involved. Using this approach, cattle BTFs can be converted to BTFs for other species by dividing the published BTF by the

fat content of a cow (25%) and multiplying the result by the fat content of the species of interest. This approach may be reasonable for extrapolating to other ruminants (cattle, sheep, goats, and deer are all ruminants), but extrapolation to nonruminants (i.e., swine) or nonmammals (chickens, ducks, geese, turkeys) is highly uncertain. As a general practice, because beef has a relatively high fat content, use of beef BTFs for other ruminants, particularly goats and deer, should result in conservative exposure estimates.

Beef and milk. BTF values for beef and cow's milk are available for inorganic elements in a number of published reviews of BTF literature (Ng et al. 1982, Baes et al. 1984, NCRP 1989, IAEA 1994). Use of values from primary studies is encouraged. Where values from published compilations are to be used, values in IAEA (1994) are preferred because they represent the most recent compilation. Values for elements not included in the IAEA report should be obtained from NCRP (1989) or Baes et al. (1984), in that order.

Specific studies on transfer of organic chemicals from food to meat or milk are limited. In the absence of specific studies, the relationship between the BTFs and octanol-water partitioning coefficient for organic chemicals derived by Travis and Arms (1988) can be used. These equations, as transformed by McKone (1994), are:

$$BTF_{food-beef} = 2.5 \text{ X } 10^{-8} K_{ow} , \quad (15)$$

$$BTF_{food-milk} = 7.9 \text{ X } 10^{-9} K_{ow} , \quad (16)$$

Sheep, swine, goats. BTFs for sheep, swine, and goats are unavailable for many chemicals. IAEA (1994) presents sheep-, swine-, and goat-specific values for 16, 18, and 7 inorganic elements, respectively. If specific studies are unavailable for a chemical, use of beef-derived BTFs is acceptable. However, the uncertainty involved in use of beef-derived values for other species should be recognized when interpreting exposure estimates and risk results.

White-tailed deer. BTFs for deer are generally unavailable. Goat values from IAEA (1994) are probably the most appropriate for use for deer because of similarities in diet and morphology. If specific studies are unavailable, use of beef-derived BTFs is acceptable. However, the uncertainty involved in use of beef-derived values for deer, which have significantly less body fat, should be recognized when interpreting exposure estimates and risk results.

Poultry and eggs. BTFs for birds are unavailable for many contaminants. Chicken and egg BTF values for some inorganic elements are available in reports by IAEA (1994) and Peterson (1983). McKone (1994) provides an equation relating K_{ow}'s for organic chemicals to food-to-egg BTFs:

$$BTF_{food-egg} = 8 \text{ X } 10^{-6} K_{ow} , \quad (17)$$

A search for specific studies should be conducted to obtain bird-specific values for other inorganic and organic chemicals. Use of beef values for birds is not acceptable.

F.4.2.2 Food ingestion rate, IR_{food}

Animal food ingestion rates are widely available in the open literature, sometimes reported as wet weight and sometimes as dry weight. Because the BTFs for plants are generally reported on a dry-weight basis, daily food intake rates should also be in dry weight. Ideally, daily food intake rates for species of interest would be obtained from local agriculture extension offices. However, if acceptable data are unavailable, default values can be obtained from reviews by Hoffman et al. (1982), IAEA (1994), or McKone (1994). IAEA (1994) provides dry-weight ingestion rates for beef and dairy cattle, sheep, goats, swine, chickens, and laying hens. Because this report provides data for most species of interest rather than just beef and dairy cattle, it is used as the source for default values suggested in Table F.2.

Food intake is driven by energy requirements. Animal size, age, activity level, reproductive condition, and environmental conditions all influence energy requirements. Extensive research on the energy requirements of beef and dairy cattle, sheep, swine, and poultry under different conditions is summarized in NRC (1987). Food intake for animals of a particular size, age, or condition can be estimated using information provided in NRC (1987).

White-tailed deer. Food ingestion rates for deer are less widely available than are those for cattle. Mautz et al. (1976) report food ingestion of 1.74 kg/d, wet weight. Assuming leaves of dicotyledonous plants, which are common deer foods, are 85% water (EPA 1993b), this translates to a dry matter intake of 0.26 kg/d.

F.4.2.3 Fraction of year on site, f_p

This parameter accounts for the period during the year in which an animal is likely to be exposed to contaminants on the site. For livestock, this is the time on pasture. In some geographic regions, animals are only on pasture for a portion of the year. The default value for beef and dairy cattle used by NCRP (1984) and DOE (1995) was 0.4, assuming animals are on pasture 4–5 months out of the year. Clearly, site-specific values are desirable as grazing practices vary considerably with geographic region.

Sheep and cattle in the Paducah, Kentucky, area are often on pasture year-round while swine and chickens are not on pasture at all (D. Wilson, McCracken County Extension Center, personal communication to A. Obery, 1995). Therefore, the recommended value for sheep and cattle in this area is 1.0.

The recommended value for swine and chickens is 0. In the Portsmouth, Ohio, area, cattle and sheep are on pasture for about 9 months and pigs are on pasture for 8 months (J. Fisher, Ohio State University Extension, personal communication to A. Obery, 1995). If pigs are younger than 8 months when slaughtered, this value should be adjusted to age at slaughter. The recommended f_p values for the Portsmouth area for cattle, sheep, and swine are 0.75, 0.75, and 0.67, respectively. Year-round grazing of cattle and sheep is common practice in the southeast (Hamby 1992), so a default value of 1.0 is recommended when site-specific data are unavailable. For pigs and chickens, which are generally raised in pens or coops and maintained on commercial feeds, time on pasture is limited, and a default of 0 is suggested.

F.4.2.4 Fraction of food from site, f_s

Supplemental feeding of livestock on pasture is a common management practice; therefore, a parameter to account for the fraction of an animal's daily food ingestion that comes from a site has been included in the animal exposure model. This is generally the fraction of the diet that is fresh pasture while an animal is on pasture for most livestock. As with f_p, site-specific values should be obtained for f_s by contacting local agriculture extension agents. In the Oak Ridge, Tennessee, area, beef cattle obtain 85–90% of their food from

pasture, and dairy cattle obtain 60% of their food from pasture (P. McCallie, Roane County Agriculture Extension, personal communication to F. Dolislager, 1995). In the Paducah, Kentucky, area, beef cattle obtain 95% of their food from pasture, and dairy cattle obtain 30% of their food from pasture (D. Wilson, McCracken County Extension Center, personal communication to A. Obery, 1995). In the Portsmouth, Ohio, area, cattle are assumed to obtain 100% of their food from pasture (J. Fisher, Ohio State University Extension, personal communication to A. Obery, 1995). Dairy cattle are unlikely to obtain 100% of their food from pasture as supplemental feeding is a standard practice. Assuming dairy practices in the Portsmouth area are similar to those near Oak Ridge, the default value recommended for dairy cattle in the Portsmouth area is also 60%. In the absence of site-specific data for sheep and goats, data for beef are the suggested defaults.

F.4.2.5 Soil ingestion rate, IR_{soil}

Soil ingestion by animals can be a significant exposure route. Animals may ingest soil incidentally during grazing or grooming activities or deliberately in search of minerals. The amount of soil ingested varies seasonally, by species, and with changing environmental conditions. Site-specific data on soil ingestion rates are generally unavailable, so values must be obtained from the literature.

Beef and dairy cattle. Soil ingestion rates for cattle are much less than 2 kg/d, and a reasonable estimate would be between 0.25 and 0.5 kg/d (Smith 1977). McKone and Ryan (1989) summarized 6 studies and report mean soil ingestion rates of 0.39 and 0.41 for beef and dairy cattle, respectively. However, Zach and Mayoh (1984) suggest that soil ingestion may range from 0.1 to 2.2 kg/d. Mayland et al. (1977) reported ingestion rates of 0.73 and 0.99 kg/d in June and August, respectively. IAEA (1994) estimates soil ingestion by grazing cattle at about 6% of dry matter intake. Assuming dry matter daily intake of 16.1 kg, daily soil ingestion would be about 1 kg. DOE (1995) used a default of 1 kg/d, and this value is also suggested as the default in this white paper.

Sheep. Sheep soil ingestion rates vary from near 0 to 27% of dry matter intake (McMurter et al. 1993). Assuming a dry matter intake of 1.3 kg/d, soil ingestion could be as high as 0.35 kg/d. However, mean soil ingestion rates reported by Fries (1982), Field and Purves (1964), and McMurter et al. (1993) were all less than 0.1 kg/d. IAEA (1994) estimates soil ingestion by grazing sheep to be 10% of daily food intake. The default value recommended for use is 0.13 (10% of 1.3 kg dry food/d).

Goats and white-tailed deer. Soil ingestion rates for goats were unavailable. However, Beyer et al. (1994) report soil ingestion by deer of <2% of diet. Assuming goat soil ingestion would be similar to that for a deer and that goat food intake is 1.3 kg dry food/d, soil ingestion by goats would be 0.03 kg/d. Assuming soil ingestion to be 2% of the diet, soil ingestion by white-tailed deer is 0.005 kg/d.

Swine. McMurter et al. (1993) report soil ingestion by pigs ranging from 1.2 to 8.0% of total dry matter intake with a mean of 4.1%. Assuming a daily food intake of 2.4 kg, soil ingestion would be 0.10 kg/d with a range of 0.05 to 0.19. The average value of 0.10 kg/d is suggested as the default soil ingestion rate for swine.

Chickens. Chickens require grit in their diet to aid digestion, and 2% grit by weight in the diet is thought to be optimum (NRC 1984). Therefore, it is assumed that soil intake by chickens is 2% of daily feed intake (McKone 1994). If daily feed intake is 0.07 kg dry food, then the soil ingestion rate for chickens is 0.0014 kg/d.

F.4.2.6 Fraction of area that is contaminated, f_a

The fraction of the site that is contaminated represents the fraction of soil ingested that is likely to be contaminated. If only half of a site is affected by contamination, presumably only half of the soil ingested would

contain contaminants. This assumes that animals graze equally over an entire pasture or site. The size of the site in relation to the amount of pasture required per animal should be considered when estimating the fraction that is contaminated. In addition, local management practices such as rotating animals from one pasture to another may influence exposures. This parameter must be determined on a site-specific basis. The default value of 1.0 is conservative and assumes the entire area is contaminated.

F.4.2.7 Water ingestion rate, IR_{water}

Animal water ingestion rates vary considerably by species, dry matter intake, body size, productivity, and environmental condition. Ideally, water ingestion rates should be obtained on a site-specific basis for each species of interest.

Beef cattle. For beef cattle, 50 L/d is commonly used as a default water ingestion rate (NRC 1977, NCRP 1984, Whelan et al. 1987, DOE 1995). IAEA (1994) lists a range of 20–60 L/d for a 500-kg beef cow. In the absence of site-specific data, 50 L/d is recommended as the default water ingestion rate for beef cattle. The water ingestion rate to be used for beef cattle in the vicinity of Paducah, Kentucky, is 37.8 L/d (D. Wilson, McCracken County Extension Center, personal communication to A. Obery, 1995).

Dairy cattle. Adequate water intake is extremely important for dairy cattle; restricting water intake decreases milk production (NRC 1989). NRC (1989) provides an equation for estimating water intake based on dry matter intake, milk production, sodium intake, and minimum daily temperature. NAS (1972) reports water intake of 90 L/d for lactating dairy cattle. NRC (1981) notes that the estimated water requirement for cattle is 3.5 to 5.5 kg of water/kg dry diet. Assuming a dry diet of 16 kg/d, this corresponds to a range of 56–88 L/d. IAEA reports a range of 50–100 L/d. The midpoint of both these ranges is about 75 L/d, and this is suggested as the default value for water intake by dairy cattle in the absence of site-specific data. Dairy cattle in the Paducah region ingest about 56.8 L/d (D. Wilson, McCracken County Extension Center, personal communication to A. Obery 1995)

Sheep. Water ingestion by sheep ranges from 4–8 L/d (NAS 1972, IAEA 1994). A value of 6 L/d is selected as the default value.

Goats. Water ingestion by goats ranges from 5–10 L/d (IAEA 1994). Bond and Straub (1975) report water intake of 8 L/d, and this is suggested as the default value for goats.

White-tailed deer. Water ingestion by deer varies with body size and environmental conditions. Lautier et al. (1988) report mean water intake of 3.61 L/d (range 1.4–13.5) for white-tailed deer. The mean value of 3.61 L/d is recommended as the default water ingestion rate for deer.

Swine. IAEA (1994) reports water ingestion rates by 110 kg pigs range from 6–10 L/d. Fattening pigs weighing 60–100 kg drink about 8 L/d (NAS 1972). Average slaughter weights of pigs in the Paducah and Portsmouth regions are about 110 kg. A default water ingestion rate of 8 L/d is suggested for pigs.

Chickens. It is generally assumed that birds drink approximately twice as much water as the amount of food they eat on a weight basis, but intake can vary substantially with environmental conditions, species, and size (NRC 1994). Daily water ingestion by chickens varies from 0.1 to 0.3 L/d (IAEA 1994). The recommended default value is 0.2 L/d (NAS 1972).

4.2.8 Fraction of daily water intake from site, f_w

The fraction of an animal's daily water intake that is obtained from water at a site should be determined on a site-specific basis. Generally, animals are assumed to obtain 100% of their water from the site (default value = 1.0) unless site conditions or management practices are known to influence access to site-related water. The reader should note that water ingested by animals may be groundwater pumped to water troughs.

F.5. SUMMARY

This report presents and describes exposure models for determining contaminant concentrations in leafy and nonleafy vegetables, beef, milk, and other animal products. In addition, default values are recommended for all model parameters (Tables F.1 and F.2). Site-specific data are preferred, but it is not always possible or practical to obtain site-specific data for all parameters. Results from the models are input directly into standard equations for estimating chronic daily intake by humans to support risk assessment efforts. While food chain exposures can be significant, they do not need to be evaluated at all sites. The ER Risk Assessment Program Manager should be consulted when determining the need for evaluating food chain exposures at a site.

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Appendix G

GUIDE FOR DETERMINING EXPOSURE UNITS

G.1. INTRODUCTION

Calculation of the contaminant concentration is an important step in the exposure modeling process and ultimately in the final risk assessment. Typically this concentration is some statistic of the available data used to represent the site contamination level. The U.S. Environmental Protection Agency (EPA) advocates the use of the upper 95% confidence limit on the mean, citing it as a reasonable exposure value (EPA 1989). Many factors can influence the calculation of the concentration; several of these factors are presented in this white paper: exposure unit size, sampling scheme, spatial correlation, temporal factors, and detection limits. Any one of these factors can severely impact an analysis and must be dealt with appropriately. This white paper presents methods and, in some cases, guideline recommendations for addressing these factors. It is important to note that each decision or estimate be technically defensible and applicable to the site being considered.

An *exposure unit* defines the physical space in which an individual will be affected by a particular contaminant (radionuclides, metals, organics, etc.) and in which the nature of the contamination can change. An example of an exposure unit could be the size of an individual's backyard. The contaminant concentration used in risk assessment usually depends on an areal average, and the exposure unit defines the area over which this average is taken. Therefore, the definition of the exposure unit has a significant effect on the risk outcome since it directly affects the contaminant concentration used in risk calculations (leading to values for carcinogenic risk, noncarcinogenic hazards, chronic daily intakes, etc.). However, it is difficult usually to quantify such unknowns as the size of a residential lot, a farm, or a recreation area. As a result, concentrations can be estimated either over- or under-conservatively.

The *sampling design* can play a significant role in calculations. From a statistical standpoint, an ideal sampling design would be a randomly distributed set of samples; however, this is rarely the case since resources are spent characterizing areas of interest to identify hotspot or plume boundaries. Such schemes are called *preferential sampling* and can severely inflate mean estimations. This white paper presents methods to compensate for this design and derive better estimations.

As mentioned previously, the upper 95% confidence limit on the mean is typically used as the representative value for contamination, which is intended to maintain a certain degree of conservatism in the analysis. However, the level of conservatism that is reported can be overstated in the presence of *spatial correlation*, which refers to the fact that contamination data are usually not completely independent observations. Applying traditional methods of analysis to such data can lead to confidence limits that are underestimated. For example, one could construct a confidence interval for the mean of correlated data that is reported as a 95% level of confidence when in reality the confidence interval is only 60%. Methods for addressing this issue to arrive at true limits are presented in this report.

The common use of *detection limits* provides limitations in interpreting environmental data. In the collection and analysis of contaminant concentrations, there is a certain level below which accurate determinations are not possible; these are usually reported as less than the detection limit (DL). From a statistical standpoint this presents a problem. Concentrations above the DL are numerical, while those below are categorical. Incorporating these measurements is important because they provide additional information. This white paper presents several methods for dealing with DLs that have had practical value in environmental applications and have been used in determining exposure concentrations.

This report addresses each of these issues, providing general guidelines and making recommendations where appropriate. The first section deals with defining exposure unit sizes using available data regarding land

use scenarios. The second section assumes that the exposure unit has been defined and presents methods for improving calculations on that exposure unit. Section G.3 addresses the problem of detection limits, while Sect. G.4 returns to defining exposure units and demonstrates how *geostatistics*, a form of spatial analysis, can be used both separately and within the framework of Sect. G.1 to define exposure units. In addition, this white paper serves to provide guidelines that will assist in many decisions.

G.2. EXPOSURE UNITS

As stated previously in Sect. G.1, an *exposure unit* defines the physical space and/or duration of time in which an individual will be affected by a particular contaminant and in which the nature of the contamination can change. The exposure unit is used in the risk assessment exposure equations to calculate the exposure concentration; therefore, the exposure unit can have a significant impact on the resulting risk estimate. Figure G.1 presents an example contamination problem (note that a lighter color denotes a lower contamination level).

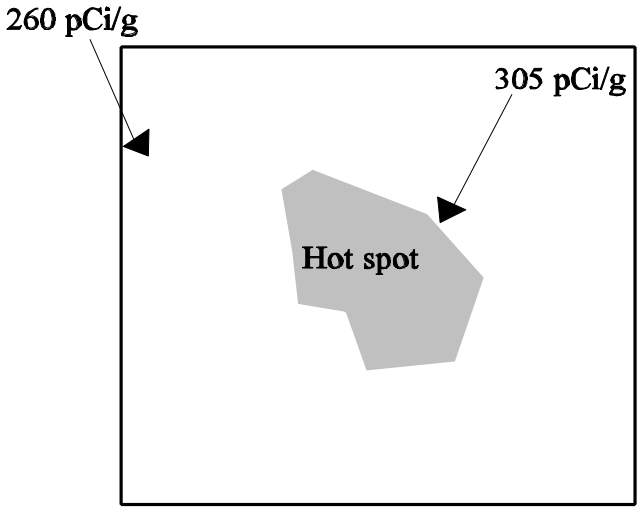

Figure G.1. Agricultural scenario

The well-defined hotspot in the center contains a maximum activity of 400 pCi/g for ^{238}U and then quickly dissipates to background. If one defines the farm size to be the area of contamination, then the mean concentration is high (305 pCi/g[1]). If one defines the farm to cover the size of the entire plot, then the mean concentration (260 pCi/g) and resulting risk level are much lower. The decision to remediate likely will change based on the farm size chosen. This assumption will hold true for each type of media (soil, sediment, groundwater, and surface water) in each pathway considered (ingestion, dermal contact, radionuclide exposure, ingestion of biota in contact with the media, etc.).

In the previous example, it is not possible that an entire agricultural scenario could be supported by a 10 ft × 10 ft land area. However, due to the difficulty in defining an alternative unit size, there is an incentive to use the most conservative approach, which can lead to an unrealistic risk assessment. A discussion of each media type is presented in the following subsections.

G.2.1 Soil

Determining the size of an exposure unit for any scenario in a soil contamination problem is an important factor in establishing the overall human health risk. While the factors contributing to the size determination are usually site specific, general issues must be addressed from site to site. This white paper seeks to clarify those issues and pose a general recommendation for an example area (particularly the Oak Ridge, Tennessee, area). The following factors are discussed:

- Three soil exposure unit scenarios
- The impact of defining the exposure unit size
- A distribution of land use sizes for the example area (Oak Ridge)
- Statistics of each land use distribution as a reasonable exposure unit size

Conditions that contribute to determining the unit size vary widely from site to site. With respect to soil contamination which is typically a slow or stationary advective process, there are three general scenarios that can occur with the definition and positioning of an exposure unit:

1. a single contamination zone within an exposure unit,
2. multiple contamination zones within an exposure unit, and
3. an exposure unit within a contamination zone.

The size of the exposure unit is the area in which the representative contamination concentration will be averaged. It is an important consideration because the larger the area, the smaller the exposure unit concentration will become eventually. Currently, the consequences of an underestimated risk calculation provide incentives to use the most conservative unit size; e.g., the area of the worst contamination. To demonstrate the influence of areal averaging, the three general scenarios, with increasing exposure unit sizes and associated unit averages, are presented in the following example.

For the first scenario, a hotspot, which is 10 ft × 10 ft with measured values of 150 pCi/g of uranium, is located in the center of the exposure unit. The exposure unit is increased in increments of 100 sq ft across clean soil outward to 800 sq ft with a length and width of approximately 28 ft as shown in Figure G.2. Figure G.3 demonstrates the resulting exposure unit concentration with each increment.

In the second scenario, multiple hotspots exist on a site. Figure G.4 illustrates how the site concentration behaves as the size of the exposure unit increases and encompasses other zones. Since the percentage of the exposure unit that is contaminated fluctuates as other zones are encountered, the effect is better reflected by presenting the length and width of the exposure unit. Note that since the unit is assumed to be a square, the length and width are equal.

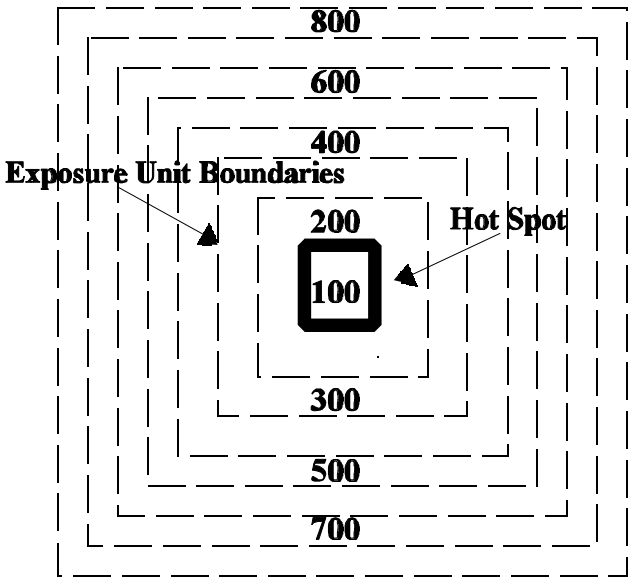

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Figure G.2. The incremental increases in unit size used for calculation in Figure 3

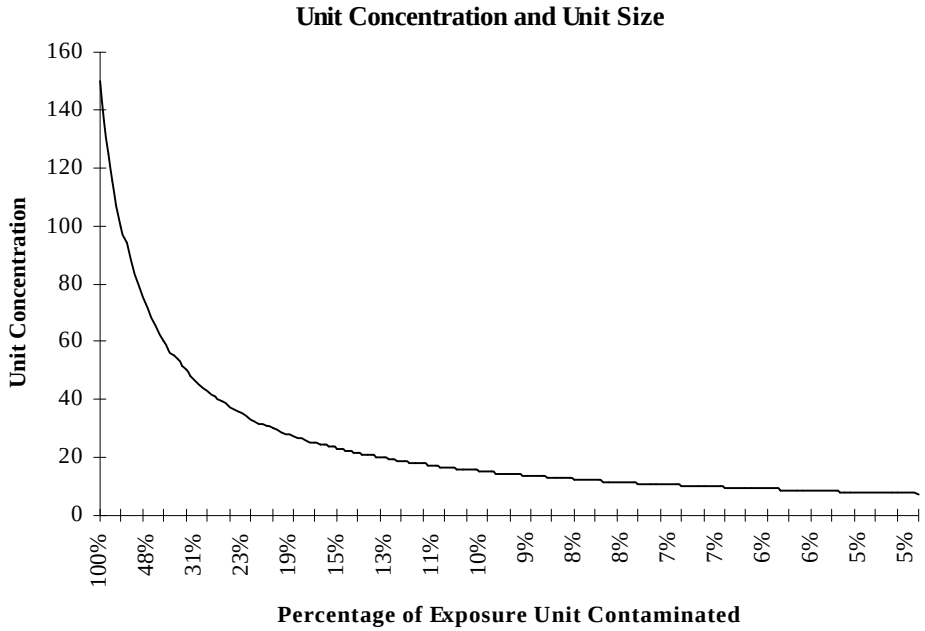


Figure G.3. Exposure concentration as a function of the percentage of the exposure unit contaminated

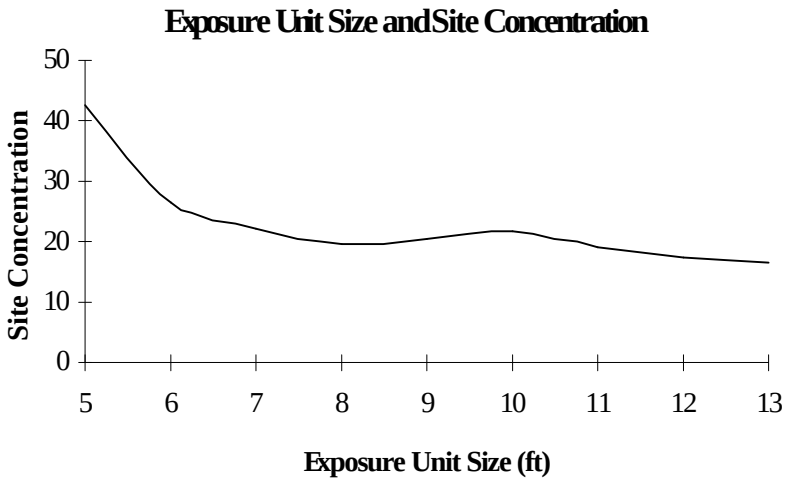


Figure G.4. Behavior of exposure concentration as unit encompasses multiple hotspots

The third scenario is similar to the first with respect to a particular exposure unit. As the unit increases or decreases, the exposure unit average can fluctuate up or down as it encounters lower and higher concentration values. The fundamental difference occurs when the following example situation is posed: Suppose that one wishes to remediate a contaminated site that is quite large. It is quite reasonable to propose that multiple exposure units could exist within the site (e.g., residential). In this example, the site has been divided into .25-acre blocks as in Figure G.5.

32	23	27	34	37	54	65	37	23	26	37	18
26	34	71	83	110	110	80	73	41	41	21	23
41	40	100	100	120	120	110	80	18	32	34	29
29	19	22	73	100	100	80	34	34	23	22	19
18	41	40	54	27	65	34	41	29	32	26	17
17	21	27	19	19	26	22	21	18	17	23	26

Figure G.5. Division of site with block average recorded in each section

At this point, two decisions about exposure unit sizes are possible. First, one can consider an exposure unit to be either of size .25 acres (equal to one of the blocks), or second, the entire site can be considered the exposure unit. The decision to remediate is set at an areal average of 50 pCi/g. In the first case, approximately 20

exposure units would have to be remediated because their block concentration exceeds 50 pCi/g. In the second case, the site would be passed as clean because the site average concentration (average of the blocks) is 44 pCi/g. Figure G.6 demonstrates the effect of exposure units on this decision rule for each decision level. The effect for both decision rules is presented when cleaning the blocks from greatest to least contaminated.

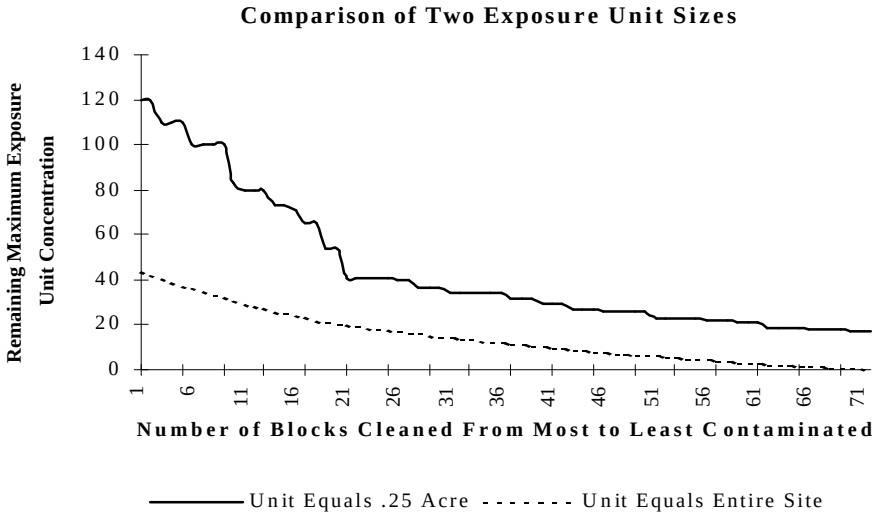


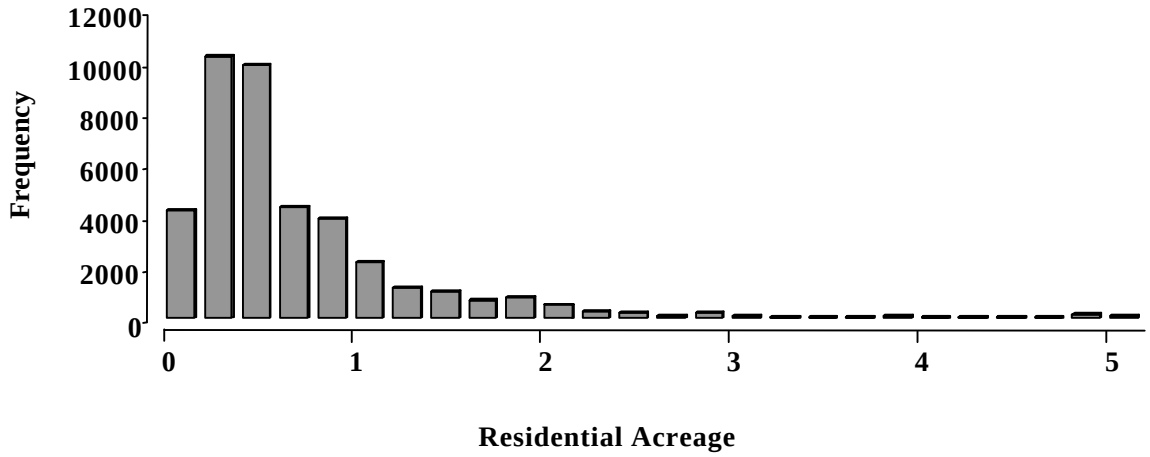
Figure G.6. Effect of exposure unit on exposure-based clean-up criteria

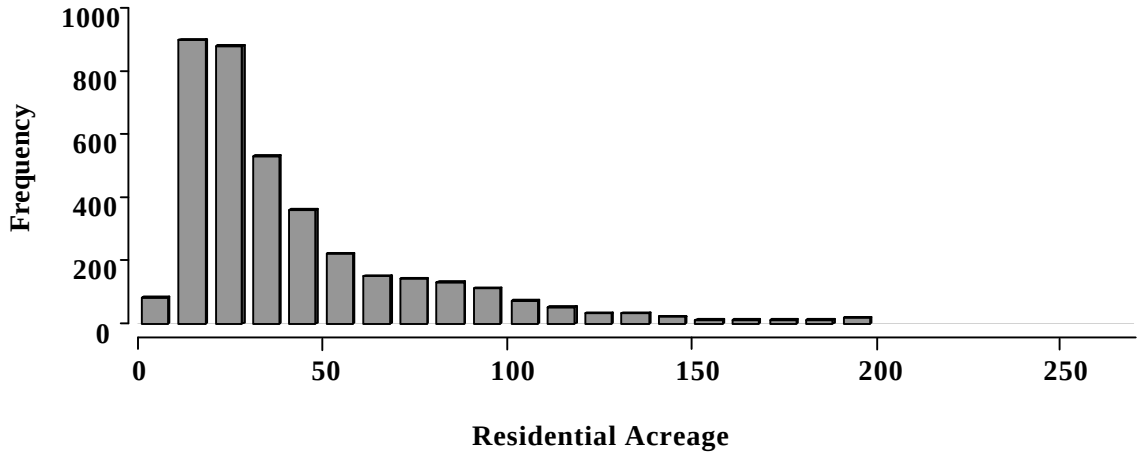
The second decision is an unlikely choice, especially for the residential scenario. However, one may argue that many houses may exist on lots larger than .25 acres.

G.2.1.1 Recommendations

To provide some insight into defining unit sizes for the local Oak Ridge area, the State Tax Assessors office was contacted, and data about property sizes for Anderson and Roane counties were assimilated. These distributions are shown in Figure G.7 and can provide a basis for determining unit sizes; however, they must be considered along with site-specific problems. As a general guideline for determining exposure unit size for areal averaging, it is recommended that the lower 5th percentile be used. It is important to note that data for recreational use were not available. The vertical size of the exposure unit is 0–2 ft for all scenarios except excavation. For the excavation scenario, 0–10 ft should be used (Miller et al. 1995). The lower 5th percentiles are as follows:

Pathway	Lower 5th percentile (acres)	Median (acres)
Residential	.16	.6
Agricultural	15	32
Industrial	.5	3.7





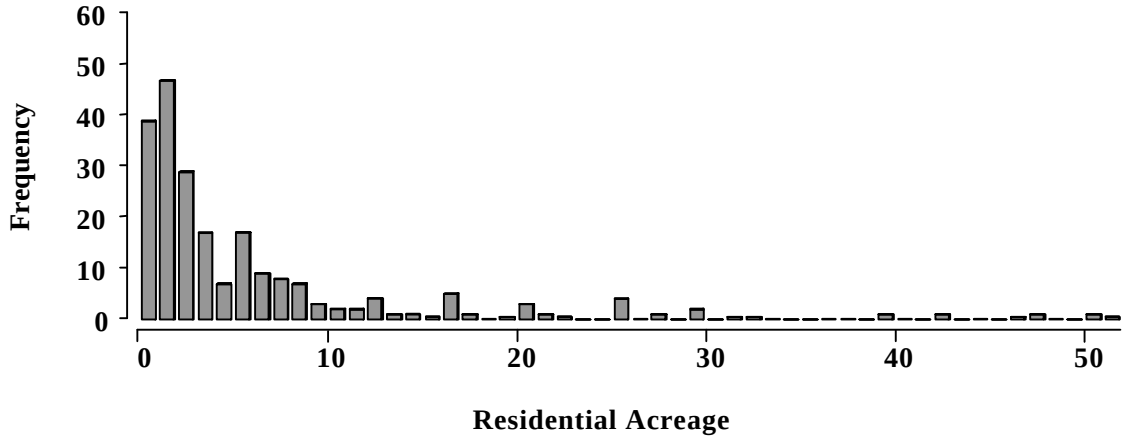


Figure G.7. Acreage by land use for Anderson and Roane counties

The purpose of defining exposure unit sizes is to provide guidance on the area to be considered for computing a contaminant concentration that a receptor will be exposed to in the above pathways. It is not meant to suggest sampling schemes. For example, adequately mapping the spread of contamination at a site may require a number of samples in a 0.16 acre plot or very few in a 15 acre plot, depending on characteristics of the site and contaminants of concern. Issues relevant to sampling schemes will be discussed in Sect. G.3.

G.2.2 SEDIMENT

An exposure unit for sediment, like soil, defines the area of sediment that a receptor is likely to contact. The same complications in calculating an exposure unit for soil apply to sediment. Consider the case of a hotspot of contamination located on the shore of a waterfront park and the recreational exposure pathway of fishing at the shoreline. Perhaps an individual consistently fishes in the area of worst contamination. The exposure unit concentration could then be the maximum concentration at the hotspot. If the receptor moves along the shore while fishing, the exposure unit will represent in large part uncontaminated sediment, and the exposure unit concentration will decrease accordingly. There is a critical difference between deriving exposure units for soil and sediment. A subsistence farm cannot be supported on a 10 ft × 10 ft section of land; however, it is not impossible for an individual to fish at the hotspot.

Determining the size of an exposure unit for consideration of human health risk from contact with sediments may not be as critical as for soil due to less time being spent in contact with sediment. For example, the yearly exposure times that the U.S. Nuclear Regulatory Commission (NRC 1977) recommends (in lieu of site specific data) for contact with sediment are:

- 12 hours, maximally exposed adult
- 8 hours, average exposed adult
- 67 hours, maximally exposed individual (all age groups)
- 47 hours, average exposed individual (all age groups)

In addition, sediment provides fewer pathways for exposure (i.e., there is no plant uptake from shoreline sediment). However, deriving reasonable guidelines for exposure unit sizes is more difficult because exposure to contaminated sediment can be highly localized. This section will discuss contact with in-place sediment through recreational scenarios only. Dredged sediment which is then spread over land areas can be treated as soil for the purpose of this analysis.

Estimation of sizes of exposure units for sediment can be done in a similar fashion as that for soil. Suggestions for determining possible exposure unit sizes for the Oak Ridge area will be presented in this section. The following topics are discussed for sediment:

- Sediment exposure unit scenarios
- The impact of determining a certain exposure unit size
- Exposure unit size recommendations

Determination of exposure unit sizes for sediment can be partitioned into the same three general exposure scenarios as for soil, although sediment contamination is potentially a much more dynamic process than soil contamination. The general situation of a park constructed (or to be constructed) along a waterbody will be used to explain each scenario. Figure G.8 presents an example recreational area.

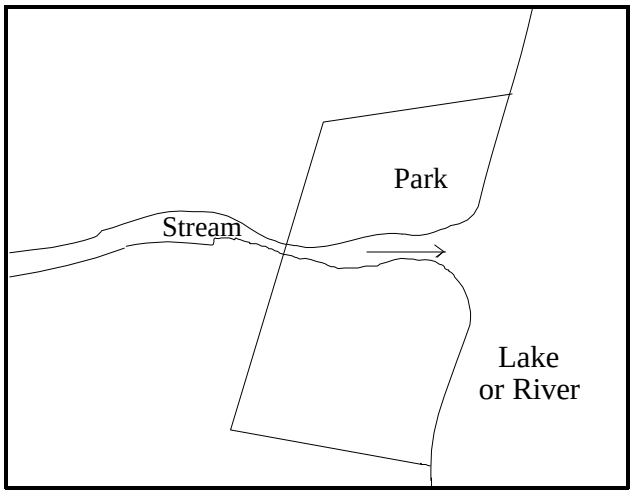


Figure G.8. Hypothetical recreational area

Exposure to sediment can occur during play (for children) or recreation (fishing) along the stream or lake shoreline. Only a very narrow band of exposed sediment will be available for contact (although more sediment would be available during very dry periods or TVA drawdowns). Figure G.9 shows that little error is introduced by assuming that sediment contaminant concentrations vary only along the shoreline direction.

Only contact with exposed sediment along the shore is being considered in this example, with risk to humans from the same direct exposure pathways as for soil (dermal exposure, ingestion, and external exposure to radionuclides). Dermal contact while swimming is usually less significant (one possible additional pathway is ingestion of sediment suspended by the action of the swimmers themselves; this pathway will not be considered herein).

Thus far, sediment exposure has been discussed as though the same contamination situations common for soils also apply to sediment. However, contamination of sediment occurs in a much more dynamic fashion than for soil. Hotspot contamination resulting from a single spill or immediate area storage leak, one of the most likely contamination situations for soil, is much less likely for sediment. Even if such a point release does occur, significant diffusion of the hotspot will occur over what could be a fairly short time frame, due to additional sediment accumulation (burying the contamination), mixing (water level variation, wave action in lakes, stream currents and eddies), and water borne diffusion. A groundwater plume, or runoff from a nearby facility, could enter a water body and cause a localized increase in the sediment contamination level. One should consider determination of exposure unit concentrations for the case of one or more localized contaminated areas (hotspots) lying along the shore within the park boundary. As the exposure unit spreads along the shoreline, additional contaminated areas are incorporated. A pattern of fluctuation in the exposure unit concentration results, as the exposure unit increases and encounters contaminated zones. Choosing all the shoreline in a park as the exposure unit may underestimate the upper percentiles of the potential exposure if contaminants are unevenly distributed.

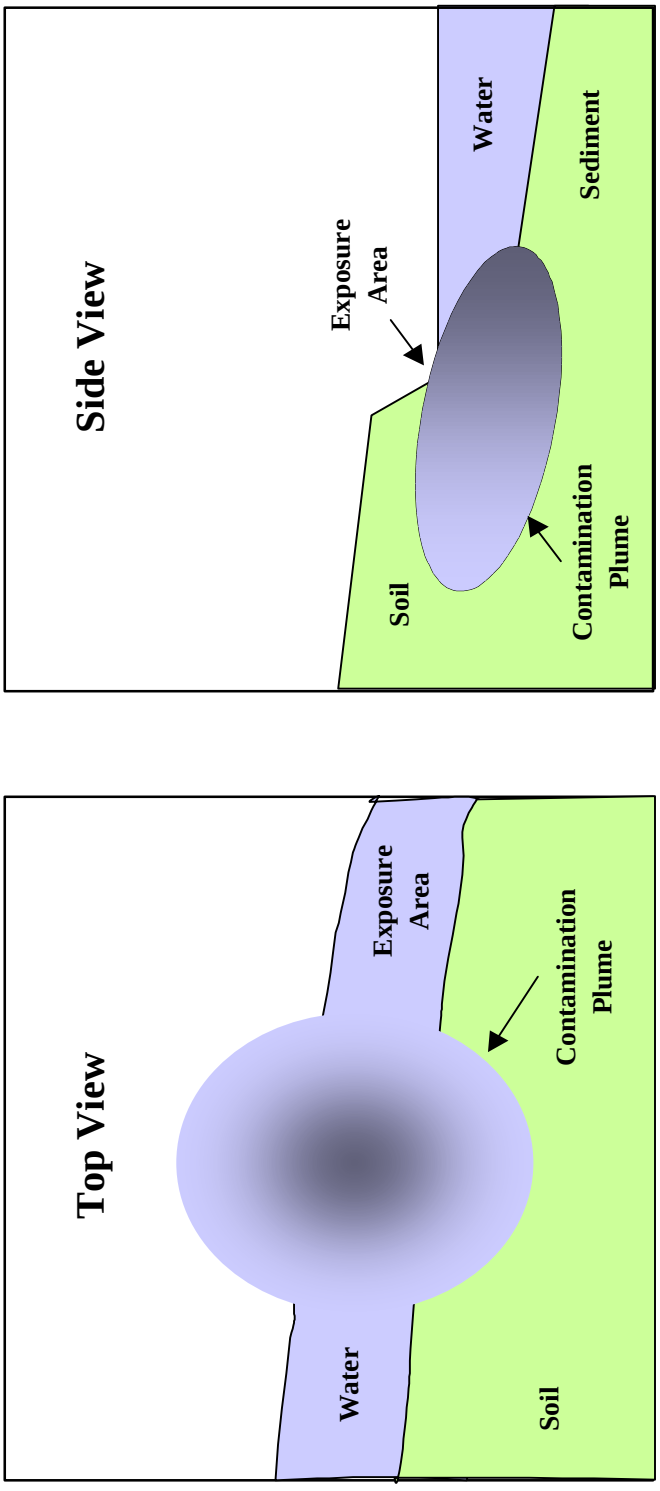


Figure G.9. Example of contaminant distribution along shoreline

More likely, contamination of sediments will result from contamination in the water column absorbing onto suspended material, which then settles out as the top layer of sediment. The source of contamination to the water could be of point or non-point (atmospheric) origin. In any case, sediment concentrations along the directly affected waterway or stream will vary gradually over space. At an intersection with another waterbody the concentrations in sediment may change greatly but then will change gradually in the new waterbody (only in the downstream direction for the case of a contaminated stream entering a river).

Contaminated sediment may be present throughout an area where more than one exposure unit may exist. An example is to consider a contaminated stream entering a lake located where there is the potential for a park to be established on the site (Figure G.10). In this case, it is likely that the contamination is the result of a contaminated water column, with concentrations that vary slowly along each waterway segment in the park (the feeder stream and the lakeshore). If the size of the park is chosen as the exposure unit, the exposure unit concentration will vary depending on the structure of the park and how much lake sediment is contained versus how much of the more contaminated stream sediment is in the park boundaries. The exposure unit concentration will vary relatively gradually with park boundary changes; this may be the most likely scenario to be encountered.

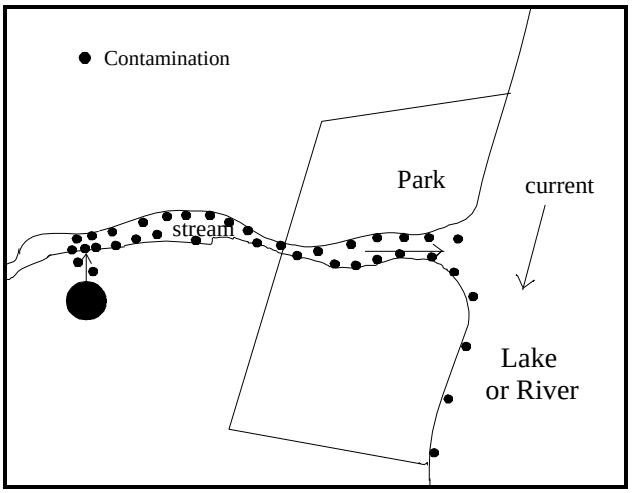


Figure G.10. Contamination scenario

It may be difficult to determine an exposure unit for sediment due to the uncertainties in recreational scenarios. As a guideline, three broad classes of sediment exposure unit scenarios are outlined in the following discussion.

In the first scenario, all the shoreline in a park is the exposure unit. This will present an opportunity to find the exposure concentration for those who jog or canvas the shoreline in low-flow conditions. Choosing all the available sediment as the exposure unit also correlates well with the most likely case of widespread contamination, as discussed previously.

In the second scenario, smaller ranges of shoreline should be defined as exposure units based on the potential for individuals to intensively use a smaller range of the shoreline. This may apply well to adult fishers, who may fish random sections adjacent to fishable waters while ignoring shorelines adjacent to small streams or shallow water. Similarly, only certain segments of the shoreline may be used for swimming. Local data may

potentially be used for this determination, if they are of sufficient detail to decide on sections of shoreline most likely to be used. For these situations, the exposure unit should be defined as a small range of the shoreline while encompassing the hotspot(s), if present. The minimum of the upper 95% confidence limit on the mean and the maximum detected concentration should again be used as the exposure concentration.

In the third scenario, assume that the highest concentration encountered will be used as the exposure unit concentration. This could be used as a worst case scenario when the most contaminated point on the shoreline is available to park users. This scenario, unlike farms entirely within tiny hot spot zones, is possible. That point on the shore could be the best fishing spot or most attractive play area for children, and it is possible (if unlikely) that these receptors may spend much of their time in one such location. In this case, no determination of the exposure unit size is needed.

Following a determination of the sediment exposure unit size and concentration, an additional step may be required to account for the spatial aspects of shorelines in the calculation of risk if using equations based on soil. To deal with the geometry of shorelines for the case of external exposure to radionuclides, the U.S. Department of Energy (DOE 1988) recommends applying dose-reduction factors for calculating exposures to photons and electrons emitted from shorelines. These factors reduce the dose one would receive from soil of an identical contaminant level. For exposure to soil, an infinite contaminated ground surface is assumed, and photons and electrons originate from all directions and distances about an individual. However, in sediment, photons and electrons originate from only a narrow band of shoreline. The dose-reduction factors account for the smaller area that emissions originate from in shoreline sediment. For photons, these factors are:

- 0.1 for a discharge canal bank,
- 0.2 for river shorelines,
- 0.3 for lake shores,
- 0.5 for ocean shores, and
- 1.0 for tidal basin.

It is important to note that as the shoreline increases in width, the risk from sediment becomes increasingly similar to that from soil. In fact, tidal basins are wide enough to be considered an infinite ground surface for external exposure to radionuclides. For electrons, it is suggested to use 1.0 as the dose-reduction factor for all shore types. Electrons have a very short range in air, so only a very small area about an individual would contribute to a dose. It is reasonable and conservative to assume that this area may not extend beyond the width of even a narrow shore, so the risk from sediment and soil are comparable for electrons. Dose reduction factors are not applicable to dermal exposure and ingestion, which are direct contact pathways.

G.2.2.1 Recommendations

Determination of sediment exposure units for recreational pathways depends not only on site characteristics but recreational behavior patterns as well. Defining the entire shoreline in a park as the exposure unit applies well to the most likely case of widespread contamination and wide-ranging (walking, jogging) activities. For varying contamination levels inside a park, using a segment of shoreline encompassing the worst of the contamination as the exposure unit is a reasonable and conservative approach, especially for patterns of activity that may not use extensive lengths of shoreline (fishing, swimming). Most conservatively, the highest level of contamination can be used as the exposure concentration. It is possible for a receptor to have a favorite shoreline spot, which could correspond to the most contaminated location.

G.2.3 Groundwater

The determination of representative exposure concentrations in groundwater presents challenges different from the other exposure media. Groundwater concentrations, like other environmental variables, are continuous over space and time. However, the difficulties of measuring groundwater at every point and the expense associated with groundwater sampling often leads to data sets that are somewhat incomplete. These uncertainties must be addressed when deriving the concentration term. Simply finding the upper 95% confidence limit on the mean for the available analytical data may not always be sufficient to support decision-making. In addition, the upper 95% confidence limit on the mean can be affected by a number of factors that affect the calculated value: the size of the defined exposure unit or plume, expected changes in contaminant concentrations over time, the degree of spatial correlation, and the location of existing wells. Often, groundwater modeling is employed to predict future exposure concentrations and account for some of these factors. The use of these models introduces other uncertainties while making unavailable the classical confidence limits used to derive the representative exposure concentration.

The drilling and use of a drinking water well or of the implementation of proposed remedial alternatives significantly affects groundwater flow characteristics which will subsequently affect the groundwater concentrations. The change in concentrations over a long period of time is significant also. The concentration often varies seasonally due to precipitation effects and also can vary over longer periods of time, often dramatically, as a contaminated groundwater plume moves into and then leaves an exposure area. The common use of groundwater modeling to account for some of these factors also can significantly influence the uncertainty in the results of a risk assessment. Although insight is gained into the potential behavior of contaminants in groundwater over time, the introduced uncertainties are often handled conservatively, resulting in exposure concentrations that significantly deviate from the upper 95% confidence limit on the mean of the currently observed concentrations. It is recommended that uncertainty analyses be performed where practical when groundwater models are used to determine exposure concentrations. The 90th percentile of the simulation results should be used as the exposure concentration to be consistent with the upper 95% confidence limit on the mean limit as recommended by EPA.

The sites of interest (Oak Ridge Reservation, Paducah Gaseous Diffusion Plant, Portsmouth Gaseous Diffusion Plant) have been known to be contaminated for many years; therefore, there are significant amounts of data at all five sites both in terms of the number of wells that have been sampled at contaminated areas and the number of times each of these wells have been sampled. This presents a problem since older data often contain a number of quality assurance difficulties (often undocumented) that may lead to spurious results. It is recommended that when historical data are used, a “moving window” be used to include data for a certain time period (e.g., the last 2 years) and that these results be periodically updated. In addition, given the large number of wells available at each of the facilities and the relatively high frequency for which they are sampled, it is recommended that groundwater risk assessment results be generated annually for all of the available data and not just for specific projects. This provides a larger scale quality assurance for the risk results that cannot be provided by laboratory records and also has the advantage of placing the risk results for a particular well or exposure unit in perspective versus the surrounding areas.

Figures G.11 and G.12 are examples of groundwater well results based on compliance data collected annually for Oak Ridge National Laboratory (ORNL). Figure G.11 demonstrates the two-dimensional well results; the size of the circle represents the magnitude of the risk, and the color of the circle shows whether the risk exceeds the EPA criteria (red), is within the range of concern (yellow), or is below the range of concern (green). Figure G.12 gives the same information in a spreadsheet format that allows one to view the

contaminants of concern. The aggregation of multiple wells for determining the exposure concentration within a contaminated area is relatively straightforward according to EPA guidance; it is recommended that the average of the representative concentration for each well (the minimum of the maximum detected concentration and the upper 95% confidence limit on the mean) be used as a representative concentration for the exposure unit. However, this does not account for any sampling bias. Two-dimensional declustering methods described later can be used to account for this bias when decision-makers are unconcerned about the variability in depth.

The most obvious difference between groundwater exposures and soil/sediment exposures is that groundwater exposures usually occur at one point within the aquifer rather than being aggregated across the entire exposure unit. At ground level, the size of an exposure unit for determining the representative exposure concentration may be the size of a single wellhead and for contaminated sites there may be more than one well available. However, the area of groundwater that is drawn by the well is much larger and often does not conform to the surface dimensions used for determining soil exposures. Generally, when determining the exposure unit for groundwater, factors such as the typical size of a farm or a residence are not as important as with the soil medium. Rather, a conceptual model for contaminant fate and transport that incorporates factors of the subsurface physical system including the properties of the aquifer system, the transport properties of site contaminants, and the relative importance of different transport mechanisms (runoff, percolation, diffusion, advection) should be employed to determine the most likely spread of contamination originating from a source. This conceptual model should be used to visualize the direction and path of the contaminants in addition to the actual or potential location of exposed receptors.

The introduction of a third spatial dimension, depth of the drinking water well, can also play an important role by increasing the variability in the potential exposure concentration. Two-dimensional geostatistical methods to account for this variability can be generalized to three dimensions but are often more difficult to implement. Definition of the exposure unit must take depth into account and define the vertical zone of interest; this is often determined by aquifer characteristics.

Another significant consideration is whether a contaminated aquifer has sufficient yield to support a drinking water well. One important modifier for the risk assessment results is the potability of the contaminated groundwater. Hydraulic conductivity, often available for wells where concentrations have been determined, can be used for the individual wells to perform a general screen of aquifer quality.

G.2.3.1 Recommendations

In summary, the calculation of risk for individual wells with analytical results is a straightforward implementation of EPA guidance; the minimum of the maximum detected concentration and the upper 95% confidence limit on the mean is used as a representative exposure concentration. This is easy to implement for a well-by-well assessment at the watershed level since no decisions are necessary regarding the aggregation of multiple wells. When the data are available for a long period of time, a moving window should be used (its length determined by the quality of the data and the presence of pronounced changes in groundwater concentrations) to parse data and provide annual updates at the watershed level. However, when groundwater data from various wells is to be aggregated (e.g., for an exposure unit for a baseline risk assessment), a number of other factors are introduced that can affect how the exposure concentration is calculated. At its simplest, the calculation of a concentration for an exposure unit involves finding the mean of each of the wells' upper 95% confidence limit on the mean. When modeling transport processes over time or modeling geostatistically over space, the 90th percentile of simulation results should be used as the exposure concentration. Caution should be exercised on basing clean-up decisions on deterministic model results without the benefit of an

uncertainty analysis.

G.2.4 Surface Water

Surface water varies more over time than space and varies as a function of groundwater conditions. Generally, the point of exposure for surface water is identified through the data quality objective process. At the watershed level, exposure points are often selected at the DOE boundary to assist in prioritization of different contributors to off-site contamination leaving via surface water. At the operable unit level, exposure points for surface water are often chosen to be the nearest impacted surface water point that could serve as a drinking water source to evaluate the potential for future land use. Contamination entering and partitioning to surface water will spread over a large area, with a relatively small variation in contaminant concentration over the length and width of the water body.

Although some contamination results from permitted direct discharges to surface water, the most likely scenario for surface water contamination resulting from past activities at DOE facilities are results from inputs of contaminated groundwater. Therefore, considerations in the determination of a groundwater exposure concentration can often be extrapolated to apply to surface water contamination. However, it is an oversimplication to consider surface water as simply diluted groundwater because the behaviors of contaminants can change greatly in the surface water environment.

Groundwater inflow is often the primary input of contamination to surface water in this scenario. However, the contaminant levels in surface water are not simply a result of dilution of contaminated groundwater. Environmental conditions in surface water are much different than in groundwater, and the chemical and environmental nature of contaminants entering a water body often change greatly when exposed to conditions present in freshwater. Organic chemicals can degrade to harmless constituents or biotransform to other hazardous compounds, which may be subjected to further transformations. Metals will be subjected to oxidizing/reducing conditions (pH, conductivity, oxygenation, etc.), various ligands will be available for complexation, and equilibrium or transformation behavior can result in transformations among different metal species, where “species” can refer to oxidation state, a ligand class, or individual metal compound. All of these processes potentially can alter the chemical behavior of the metal. Conditions may favor partitioning of dissolved pollutants and radionuclides present in the groundwater inflow to sediment or suspended material. Bodek et al. (1988) present further details on the changes pollutants are subjected to upon entering different environmental conditions.

It is important that seasonal variability be factored into any derivation of exposure concentrations for a surface water point and that this concentration represent an integrated annual average or confidence limit. Although surface water concentrations are often a function of groundwater inputs, they are not always positively correlated. It is conceivable that during time periods of high groundwater concentrations, higher surface water concentrations may not result because of increased runoff from other areas that dilute surface water concentrations. Changes in surface water concentrations over time must be considered separately from variations in groundwater concentrations, despite their direct link. Contaminant concentrations in surface water will change seasonally even if there is a steady-state level of contamination present. As precipitation, water temperature, clarity, and oxygen level vary, different chemical forms (ligands, oxidation state) of the pollutant may be favored. These different forms may have different toxicities (i.e., methylmercury and inorganic mercury, arsenic +5 and arsenic +3, etc.) or differing sorption behaviors. A contaminant may partition to the sediment at some time during the year only to desorb to the water column under later conditions. Such changes may not be gradual; lake turnover radically alters lake characteristics in a matter of hours and days.

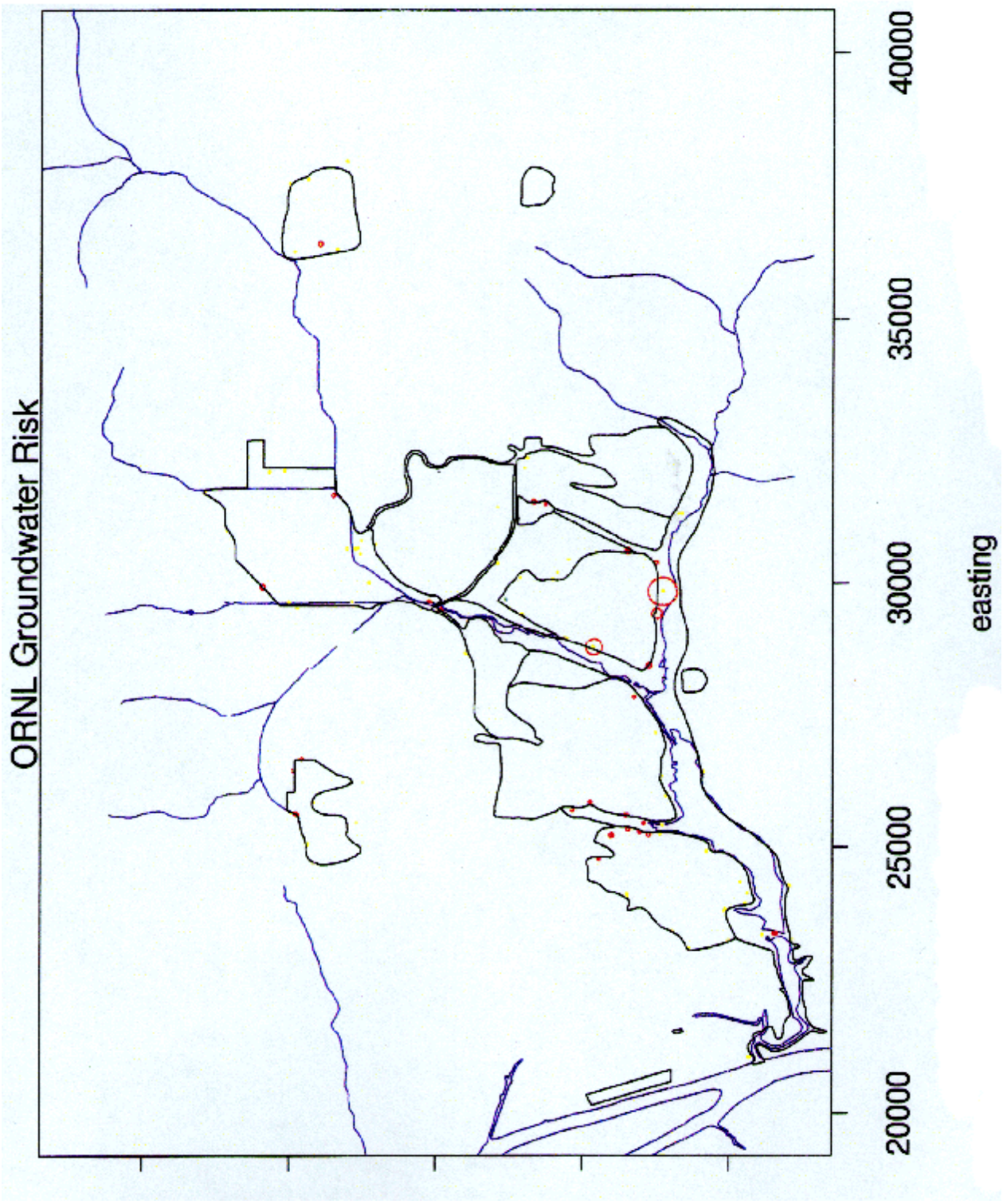


Figure G.11. ORNL groundwater risk

WELL	WAG	DCEE11	DCE12	BENZENE	CARBON_T	CHLOROFO	TRICHLOR	VINYL_CH	CO_60	CS_137	TOTAL_SR	TRITIUM	BE	BIS_2_ET	U_234	U_235	U_238	TC_99	%RAD	%MET	%TRU	%ORG	Total Risk
980	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.82E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	1.82E-06
964	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.34E-06	0.00E+00	0.00E+00					100	0	0	0	1.34E-06
963	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.06E-07	0.00E+00	0.00E+00					100	0	0	0	4.06E-07
843	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.22E-06	0.00E+00	0.00E+00	2.31E-03							100	0	0	0	2.32E-03
1243	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.72E-05	0.00E+00	0.00E+00	2.15E-03							100	0	0	0	2.23E-03
1242	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.06E-04							100	0	0	0	4.06E-04
842	6	0.00E+00	1.94E-05	0.00E+00	7.59E-05	7.94E-06	4.19E-05	0.00E+00	6.22E-06	0.00E+00	0.00E+00	8.52E-05							38.86	0	61.34	0	2.37E-04
844	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.83E-04							100	0	0	0	1.83E-04
847	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.70E-04							100	0	0	0	1.70E-04
1244	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.05E-05	0.00E+00	5.08E-06	4.87E-05	0.00E+00	0.00E+00					100	0	0	0	1.34E-04
841	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.47E-06	0.00E+00	0.00E+00	1.14E-04							100	0	0	0	1.16E-04
839	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.81E-05							100	0	0	0	3.81E-05
838	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.53E-05							100	0	0	0	3.53E-05
835	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.78E-06	1.66E-05							100	0	0	0	1.84E-05
840	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.81E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.17E-06	1.34E-05							96.61	0	3.39	0	1.71E-05
859	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.17E-06	7.71E-06							100	0	0	0	1.09E-05
836	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.12E-06							100	0	0	0	8.12E-06
837	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.28E-06							100	0	0	0	5.28E-06
833	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.44E-06	0.00E+00							100	0	0	0	4.44E-06
1245	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.81E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	3.81E-06
831	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.69E-06							100	0	0	0	3.69E-06
745	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.76E-06							100	0	0	0	2.76E-06
857	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.15E-06							100	0	0	0	2.15E-06
855	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.74E-06							100	0	0	0	1.74E-06
856	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.61E-06	0.00E+00	0.00E+00	0.00E+00							100	0	0	0	1.61E-06
858	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.61E-06	0.00E+00	0.00E+00	0.00E+00							100	0	0	0	1.61E-06
832	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E-06	0.00E+00							100	0	0	0	1.40E-06
860	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.52E-07							100	0	0	0	8.52E-07
1079	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.61E-05	1.97E-06	4.12E-06	8.49E-04	0.00E+00	0.00E+00				7.47E-07	100	0	0	0	8.72E-04
1078	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.61E-04	5.20E-06	6.98E-06	5.28E-05	0.00E+00	0.00E+00				2.62E-04	100	0	0	0	4.38E-04
1076	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.76E-06	4.08E-04	0.00E+00	0.00E+00					100	0	0	0	4.11E-04
1084	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.90E-06	0.00E+00	3.81E-06	1.22E-04	0.00E+00	0.00E+00				5.40E-06	100	0	0	0	1.34E-04
1074	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.44E-06	4.87E-07	1.20E-04	0.00E+00					3.95	96.05	0	0	1.25E-04
1082	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.60E-05	0.00E+00	0.00E+00					100	0	0	0	2.60E-05
1083	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.71E-06	1.08E-05	0.00E+00	0.00E+00				1.59E-06	100	0	0	0	1.79E-05
1080	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.61E-06	0.00E+00	3.17E-06	2.80E-06	0.00E+00	0.00E+00					100	0	0	0	7.38E-06
1085	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.44E-06	8.52E-07	0.00E+00	0.00E+00					100	0	0	0	5.29E-06
1075	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.61E-06	0.00E+00	1.84E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	3.45E-06
1077	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.74E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	1.74E-06
1081	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E-06	0.00E+00	0.00E+00					100	0	0	0	1.01E-06
1071	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.74E-07	0.00E+00	0.00E+00					100	0	0	0	9.74E-07
1096	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.41E-03	0.00E+00	0.00E+00	0.00E+00					99.96	0	0.04	0	2.41E-03
1087	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.72E-06	0.00E+00	6.56E-04	9.33E-07	0.00E+00						100	0	0	0	6.69E-04
1097	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.86E-05	1.61E-06	0.00E+00	0.00E+00	1.27E-04	0.00E+00	0.00E+00	0.00E+00					62.05	0	37.95	0	2.07E-04
1088	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.33E-05	0.00E+00	0.00E+00					100	0	0	0	9.33E-05
1092	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.07E-06	0.00E+00	1.59E-06	5.28E-06	0.00E+00	0.00E+00					100	0	0	0	7.93E-06
1095	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.87E-06	1.14E-06	0.00E+00	1.00E-06					75.01	0	24.99	0	4.01E-06
1094	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.98E-06	0.00E+00	0.00E+00					100	0	0	0	3.98E-06
1090	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.85E-06	0.00E+00	0.00E+00						100	0	0	0	1.85E-06
1091	8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.10E-06	0.00E+00	0.00E+00					100	0	0	0	1.10E-06
1143	11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.98E-06	0.00E+00	1.72E-06	0.00E+00	2.38E-06	0.00E+00	0.00E+00	0.00E+00					45.15	0	54.85	0	9.07E-06
1148	11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.44E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	2.44E-06
1139	11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.25E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	2.25E-06
1246	11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.46E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	1.46E-06
1201	17	2.52E-04	0.00E+00	8.19E-06	0.00E+00	0.00E+00	2.25E-03	3.83E-03	0.00E+00	0.00E+00	6.86E-06	8.52E-06	0.00E+00	0.00E+00					0.24	0	99.76	0	6.46E-03
1198	17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.49E-06	1.38E-05	0.00E+00	0.00E+00					100	0	0	0	1.73E-05
1199	17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.90E-06	0.00E+00	2.92E-06	1.14E-05	0.00E+00	0.00E+00					100	0	0	0	1.72E-05
1203	17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.30E-06	5.28E-06	0.00E+00	0.00E+00					100	0	0	0	1.26E-05
1200	17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.12E-06	8.12E-06	0.00E+00	0.00E+00					100	0	0	0	1.22E-05
1202	17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.31E-06	0.00E+00	0.00E+00	0.00E+00	6.86E-06	3.04E-06	0.00E+00	0.00E+00					88.11	0	11.89	0	1.10E-05
1197	17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.79E-06	0.00E+00	0.00E+00	4.48E-06	0.00E+00	0.00E+00					100	0	0	0	7.25E-06
1196	17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.50E-06	0.00E+00	0.00E+00	5.28E-06	0.00E+00	0.00E+00					100	0	0	0	6.78E-06

Figure G.12. ORNL groundwater risk spreadsheet

WELL	WAG	DCEE11	DCE12	BENZENE	CARBON_T	CHLOROFO	TRICHLOR	VINYL_CH	CO_60	CS_137	TOTAL_SR	TRITIUM	BE	BIS_2_ET	U_234	U_235	U_238	TC_99	%RAD	%MET	%TRU	%ORG	Total Risk
812	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.86E-06	6.81E-07	0.00E+00	2.25E-06	0.00E+00	6.88E-03	4.87E-06	0.00E+00	0.00E+00	3.92E-04	2.67E-06	1.27E-05		95.42	0	4.55	0.04	6.93E-03
825	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.23E-04	0.00E+00	0.00E+00	3.17E-06	1.01E-06	0.00E+00	0.00E+00					0.5	0	0	99.5	8.29E-04
806	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.66E-04	1.26E-06	0.00E+00	0.00E+00					100	0	0	0	1.86E-04
830	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.49E-05	2.11E-05	0.00E+00	0.00E+00					100	0	0	0	5.60E-05
946	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.06E-05	1.82E-06	0.00E+00	0.00E+00					100	0	0	0	2.22E-05
829	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.29E-06	0.00E+00	1.81E-05	1.74E-06	0.00E+00	0.00E+00					100	0	0	0	2.11E-05
947	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.23E-06	0.00E+00	1.70E-05	0.00E+00						100	0	0	0	2.03E-05
818	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.69E-06	0.00E+00	1.46E-05	0.00E+00	0.00E+00					100	0	0	0	1.73E-05
821	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.11E-06	0.00E+00	2.36E-06	3.94E-06	0.00E+00	0.00E+00					100	0	0	0	1.47E-05
823	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.08E-05	3.86E-06	0.00E+00	0.00E+00					100	0	0	0	8.93E-06
811	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.06E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	5.06E-06
810	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.88E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	8.88E-06
820	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.90E-06	2.15E-06	1.71E-06	2.03E-06	0.00E+00	0.00E+00					100	0	0	0	8.79E-06
815	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.39E-06	2.39E-06	0.00E+00	0.00E+00					100	0	0	0	7.79E-06
816	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.30E-06	2.36E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	6.68E-06
821	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.11E-06	0.00E+00	3.17E-06	0.00E+00	0.00E+00						97.15	0	0	2.85	6.47E-06
822	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.55E-06	4.87E-06	0.00E+00	0.00E+00					100	0	0	0	6.42E-06
809	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.12E-06	2.19E-06	0.00E+00	0.00E+00					100	0	0	0	6.32E-06
807	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.81E-06	2.43E-06	0.00E+00	0.00E+00					100	0	0	0	6.24E-06
819	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.04E-06	0.00E+00	1.90E-06	2.07E-06	0.00E+00	0.00E+00					100	0	0	0	6.01E-06
808	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.82E-06	0.00E+00	3.81E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	5.63E-06
827	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.90E-06	1.54E-06	0.00E+00	0.00E+00					100	0	0	0	3.45E-06
814	1	0.00E+00	0.00E+00	2.13E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.18E-06	0.00E+00	0.00E+00					35.58	0	0	64.42	3.31E-06
828	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.03E-06	0.00E+00	0.00E+00					100	0	0	0	2.03E-06
1191	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.90E-06	0.00E+00	4.12E-04	2.72E-04	0.00E+00	0.00E+00					100	0	0	0	6.87E-04
1190	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.71E-06	1.01E-04	0.00E+00	0.00E+00					100	0	0	0	1.07E-04
1186	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.92E-05	1.34E-06	0.00E+00	0.00E+00					100	0	0	0	3.06E-05
1192	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.13E-06	8.88E-06	1.06E-05	0.00E+00	0.00E+00					100	0	0	0	2.36E-05
1187	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.35E-05	2.47E-06	8.52E-07	0.00E+00	0.00E+00					100	0	0	0	1.68E-05
1188	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.38E-06	1.21E-05	1.82E-06	0.00E+00	0.00E+00					100	0	0	0	1.51E-05
1194	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.43E-06	3.77E-06	1.59E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	8.79E-06
1195	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.04E-06	0.00E+00	3.81E-06	1.01E-06	0.00E+00	0.00E+00					100	0	0	0	6.86E-06
1189	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.81E-06	3.90E-06	0.00E+00	0.00E+00					100	0	0	0	5.70E-06
994	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.77E-06	7.61E-04	3.08E-05	0.00E+00	0.00E+00					100	0	0	0	7.96E-04
993	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.49E-04	1.87E-05	0.00E+00	0.00E+00					100	0	0	0	3.68E-04
996	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.77E-04	1.07E-06	1.52E-06	5.39E-06	2.03E-06	0.00E+00	0.00E+00					5.36	0	0	94.64	1.87E-04
986	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.61E-04	0.00E+00	0.00E+00	0.00E+00	2.31E-06	0.00E+00	0.00E+00					1.42	0	0	98.58	1.63E-04
992	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.50E-06	0.00E+00	6.68E-06	1.83E-06	0.00E+00	0.00E+00					100	0	0	0	7.00E-06
997	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.29E-06	0.00E+00	3.49E-05	1.54E-06	0.00E+00	0.00E+00					100	0	0	0	3.77E-05
991	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.30E-06	5.08E-06	1.87E-06	0.00E+00	0.00E+00					100	0	0	0	1.12E-05
985	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.30E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.52E-06	0.00E+00	0.00E+00					52.2	0	0	47.8	4.82E-06
990	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.06E-06	1.79E-06	0.00E+00	0.00E+00					100	0	0	0	3.85E-06
998	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.49E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	3.49E-06
988	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.97E-06	1.26E-06	0.00E+00	0.00E+00					100	0	0	0	3.23E-06
995	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.50E-06	0.00E+00	0.00E+00					100	0	0	0	1.50E-06
987	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.42E-06	0.00E+00	0.00E+00					100	0	0	0	1.42E-06
973	4	0.00E+00	6.00E-06	6.30E-07	0.00E+00	9.17E-07	7.47E-04	0.00E+00	0.00E+00	0.00E+00	2.09E-04	3.86E-01	0.00E+00	0.00E+00					99.85	0	0.15	0	3.86E-01
974	4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.49E-05	8.54E-02	0.00E+00	0.00E+00					100	0	0	0	8.54E-02
971	4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.03E-06	1.82E-03	0.00E+00	0.00E+00					100	0	0	0	1.83E-03
972	4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.49E-06	1.83E-05	0.00E+00	0.00E+00					100	0	0	0	1.98E-05
953	4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.68E-06					0	0	100	0	7.68E-06
952	4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.25E-06	0.00E+00	1.62E-06	0.00E+00	0.00E+00	0.00E+00					100	0	0	0	3.87E-06
978	5	7.30E-05	0.00E+00	2.14E-05	0.00E+00	0.00E+00	1.54E-05	1.91E-01	0.00E+00	1.51E-05	0.00E+00	6.49E-05	0.00E+00	0.00E+00					0.04	0	0	99.96	1.91E-01
969	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.50E-06	0.00E+00	0.00E+00	5.56E-06	8.35E-04	1.45E-02	0.00E+00	0.00E+00					99.96	0	0.04	0	1.51E-02
977	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.89E-07	0.00E+00	0.00E+00	1.97E-06	9.20E-06	7.30E-03	0.00E+00	6.68E-07					99.98	0	0.02	0	7.32E-03
970	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.06E-06	1.22E-03	0.00E+00	0.00E+00					100	0	0	0	1.22E-03
981	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.71E-05	0.00E+00	0.00E+00					100	0	0	0	7.71E-05
979	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.79E-06	0.00E+00	4.46E-05	0.00E+00	0.00E+00					100	0	0	0	5.34E-05
968	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.00E-06	3.95E-06	0.00E+00	2.52E-06	0.00E+00	1.10E-05					46.2	0	0	53.8	2.05E-05
983	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.07E-06	0.00E+00	0.00E+00	8.93E-06	0.00E+00	2.67E-06					78.91	0	0	21.09	1.27E-05
965	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.03E-06	1.30E-06	0.00E+00	0.00E+00					100	0	0	0	7.33E-06
984	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.35E-06	0.00E+00	0.00E+00						100	0	0	0	6.35E-06
966	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.89E-06	0.00E+00	0.00E+00	1.79E-06	0.00E+00	0.00E+00					100	0	0	0	4.68E-06
967	5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.25E-06	1.91E-06	0.00E+00	0.00E+00					100	0	0	0	4.16E-06

Figure G.12. (continued)

G.2.4.1 Recommendations

After selection of the point of surface water exposure (usually through the data quality objective process), a sampling plan must be designed that accounts for temporal variations in surface water contaminant concentrations. Calculating the average and upper 95% confidence limit on the mean of the samples taken should provide a reasonable estimate of the surface water exposure concentration if the samples have been taken at regular intervals throughout the year. If regular sampling throughout the year is not an option (either due to time constraints or because available historical data are being used), then the data should be time-weighted to give an accurate estimate of the actual exposure concentration over time. For direct contact pathways, the seasonal data can be weighted with the fraction of time spent in recreational activities on the lake in that season. Such considerations do not apply to drinking water supplies from water bodies. For recreational pathways, an improved concentration may be derived by weighting the temporal data with seasonal recreation behavior data.

G.3. EXPOSURE CALCULATIONS

Having considered the spatial and temporal aspects of defining an exposure unit, the available data for the exposure unit must then be employed to compute the required areal and temporal average contaminant concentration to complete this first step in the risk assessment process.

Data samples provide a sparse image of the spread of contamination. The role of a statistical analysis is to summarize the available data, make inferences about the site as a whole, and assess uncertainty. In the case of exposure assessment, the role of the analysis is to produce a concentration value that is representative of the entire site or subset of interest. To make statistical inferences about the site from the data, one must make certain assumptions about distribution of contamination as a whole by choosing a model to quantify the contamination. The assumptions can be driven and supported by the data or they may arise from defensible arguments such as past experiences or known site conditions. A common statistical approach is to assume that the exhaustive data set is either normally or lognormally distributed and that samples are both randomly selected and uncorrelated with each other. These assumptions are powerful tools that can drastically simplify the analysis. However, when conditions deviate significantly, continuing to maintain such assumptions can severely degrade the quality of the analysis.

Environmental contamination possesses properties that typically do not correlate with these simplifying assumptions. Assumptions of normality or lognormality have been found to hold true in many earth science applications and have therefore become general guidelines when in doubt about a particular site. There are, however, many situations where this assumption fails, and any model built on this platform is likely to be in error.

Due to budgeting constraints, the number of samples is limited, and there is incentive to move from a random sampling scheme to a scheme that will provide the greatest amount of information near or around areas of known or suspected contamination. These schemes are highly *preferential*, providing a clear image of the contamination in small areas and leaving the rest of the site sometimes inadequately represented. Ignoring preferential sampling can lead to exaggerated concentration values.

Rarely are data samples completely uncorrelated. Contamination occurs over space and time as the result of physical phenomena. These phenomena are usually not random events and therefore the distribution of contamination is not entirely random. Instead, the data are often *spatially correlated*. In the presence of spatial

correlation, the degree to which data are alike is a function of distance and direction. For example, data that are closer together are often more alike than data taken further away. In many cases, data in a certain direction tend to be more alike than in another such as in a contaminant plume.

This section will provide practical solutions for dealing with data that deviate from assumptions of normality, independence, and random design. The effect of these deviations will be explained and demonstrated. The emphasis of the analysis will be to arrive at an improved representative concentration that will produce a better estimate of exposure to individuals on the site. Before any statistical considerations are discussed, we now introduce the data, the conditions surrounding the site, and the ultimate goal of the analysis.

G.3.1 Description of the Example

This example is derived from a data set taken from a site in the Oak Ridge area. An exhaustive representation of contamination across the site is shown in Figure G.13.

From this data set, 84 samples were taken with their location and magnitude as shown in Figure G.13. It is clear from this sampling scheme that there are at least two areas of high contamination, both of which have been heavily sampled. The remaining data do not show the presence of another hotspot. For simplification, the exposure unit is defined to be the entire study area. The goal of the study is to determine a concentration value for the entire site that will be a good representation of the effective concentration an individual will be exposed to over a given length of time.

To further simplify the analysis, it is assumed that the individual will be exposed equally and randomly to all points in the unit. This is a reasonable assumption particularly in the absence of development plans. The mean concentration over the entire site is therefore the representative statistic. Others can be used as well, such as the median or the upper 95th percentile. For situations where this assumption is not valid, weights that reflect a bias in exposure frequency should be included in the analysis. The assignment of these weights is site specific but would be applied in the same fashion as weighting schemes presented later in this white paper. In addition to stating the representative concentration, it is important to assess the uncertainty associated with that value.

Four levels of analysis will be conducted from the traditional approach to geostatistical tools of simulation. The effect of each analysis will be explained both in statistical terms and demonstrated in terms of the concentration term. For demonstration purposes, the two-sided 95% confidence interval on the mean will be used.[1]

Before the analysis begins, note that the following information is available from the exhaustive data set: the mean and standard deviations of the exhaustive data are 216 and 62 pCi/g, respectively. The exhaustive set appears somewhat normally distributed in Figure G.13 and ranges from 69 to 396. This information is typically unavailable in the exposure assessment and is included here only to demonstrate the accuracy of each analysis. However, each analysis will be conducted based only upon information from the available data.

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[1] Traditional risk assessment uses the single sided upper 95% confidence limit on the mean. The methods presented in this section would apply in the same manner. A simple adjustment of the Z-score from 1.96 to 1.645 is all that is required.

G.3.2 Traditional Approach

The first step was to observe the histogram of sample values. Despite the non-normal appearance of the data, it will be assumed that the distribution of values is normal and that the current histogram is distorted by the preferential sampling. One could as easily assume log-normality, and the following analysis would apply with modifications.

To simplify the analysis, the fact that samples are located preferentially, as well as correlated spatially, is ignored. Under these assumptions, the limits are constructed from the mean $\bar{x}$ and the sample standard deviation s and written:

$$\bar{x} \pm 1.96\frac{s}{\sqrt{n}} \quad ,$$

where

$$\bar{x} = \frac{1}{n}\sum_i^n x_i \, , \quad s = \sqrt{\frac{1}{n-1}\sum_i^n (x_i - \bar{x})^2} \quad .$$

The sample mean of 282 pCi/g and a standard deviation of 81 pCi/g produces a confidence interval of $265 < 282 < 300$ pCi/g.

The analysis has produced a mean that is excessively high due primarily to the preferential sampling around the hotspots. Note that the true mean (216 pCi/g) is not within this confidence interval. In addition, it is reasonable to believe that the confidence limits are too strict given that spatial correlation has been ignored.

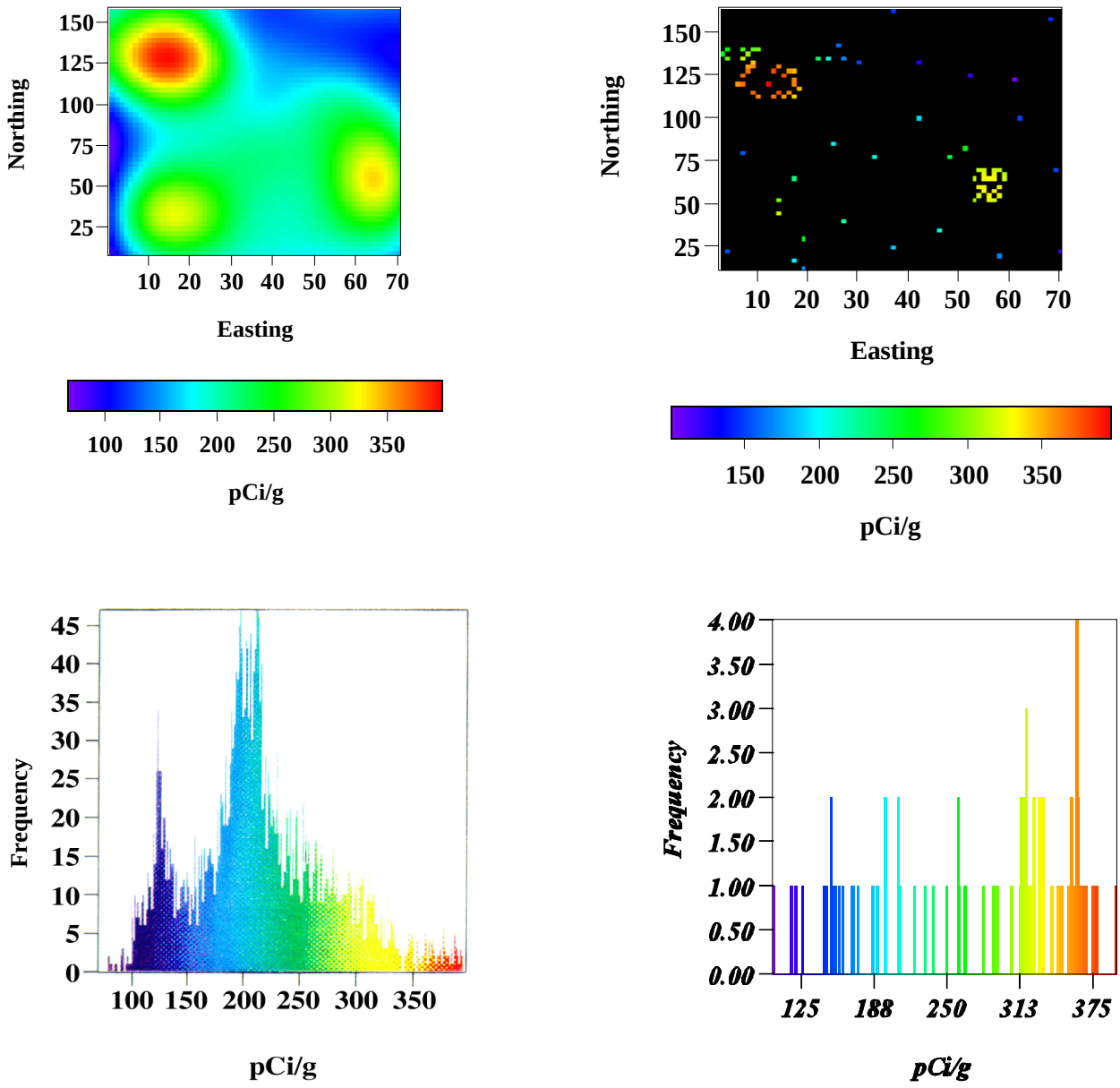

Figure G.13. The exhaustive data and sampled data with associated histograms

G.3.3 Division of Data and the Bonferroni Method

A simple way of dealing with the issue of preferential sampling is to divide the data into three sets. The first set is the cluster of data shown in the upper left hand corner of Figure G.13 and will be referred to as hotspot #1. The second set of data is the other clustered sample shown in Figure G.13 and will be called hotspot #2. The third grouping of data consists of everything else. Within each section, the data are no longer preferentially sampled, i.e., no subset of points in any section are more clustered than any other. As an added bonus, the histogram of values within each section appear more normal.

The goal is to construct the global mean and associated confidence interval. To make a statement about the global mean and assign a confidence limit, we need to invoke the Bonferroni principle (Neter and Wasserman 1974). The Bonferroni theorem states that if there are k intervals of confidence (1 - α/2k) 100% then there is a probability of at least (1 - α) 100% that they hold simultaneously. Note that the confidence limit is reduced for each confidence interval added. From a probabilistic standpoint, this implies that there is at least a (1-α) 100% confidence level that the average of the three estimates falls between the average of the upper confidence limits and the average of the lower confidence limits. To compensate for the fact that each of the subsections is not of equal size, one can weight them according to the area within each subsection. Dividing the weights by the total area normalizes the weights to one. The general equation for the global confidence limit is then written as:

$$\left(w_1L_1 + w_2L_2 + \ldots + w_kL_k < w_1\overline{x_1} + w_2\overline{x_2} + \ldots + w_k\overline{x_k} < w_1U_1 + w_2U_2 + \ldots + w_kU_k\right) ,$$

where L_i and U_i , respectively, are the lower and upper (1 - α/2k) 100% confidence limits, $\bar{x}_i$ is the local mean, w_i is the weight assigned to the ith subsection, and $\sum_i^k w_i = 1$.

To achieve at least a 95% confidence limit on the global mean, the local confidence intervals must be increased to 98.3%. The following table shows the confidence intervals and associated weights.

Region	LCL 98.3% (pCi/g)	Mean (pCi/g)	UCL 98.3% (pCi/g)	Weight
Hotspot #1	319	323	327	.021
Hotspot #2	353	361	368	.031
Remaining Area	180	205	230	.948

Applying the Bonferroni principle to these intervals results in a 95% confidence limit for the mean of 188 < 212 < 236; this is a much improved interval that now includes the true mean. The change in the interval reflects the more realistic influence that the clusters of data should have on the global statistics. However, this approach to analysis still presents several problems:

1. The subdivision of the site is arguably arbitrary. A different sectioning could produce significantly different weights. In addition, by defining the section boundaries, one is already making at least an indirect statement about the spatial extent of contamination.

2. The Bonferroni method provides only a lower bound on the confidence limits. The global confidence interval could be correct more than (1 - α) 100% of the time (Neter and Wasserman 1974).

3. The larger the number of confidence intervals, the larger the confidence interval. For a large number of confidence intervals, the confidence coefficient is too wide to be of much use. This limits the practical use of the Bonferroni method to a small number of subdivisions.

4. Spatial dependence has still not been directly addressed and could still be deflating confidence limits.

5. The data set must be large enough to subdivide.

G.3.4 Formal Declustering Analysis

Clustered data sets are essentially data that are spatially preferentially sampled. As seen in the first level of analysis, such data may not represent global parameters of the site. The idea of *declustering* the data is rather intuitive. Any declustering method seeks to weight the data according to how much of the site they should represent. The method of subdividing the data and using the Bonferroni method is essentially an ad hoc method of declustering. Data that are taken close together in space typically do not contribute any "new" information. These samples should be weighted less that those that are sampled more sparsely. Two common methods of declustering are the *polygonal method* and *cellular declustering*.

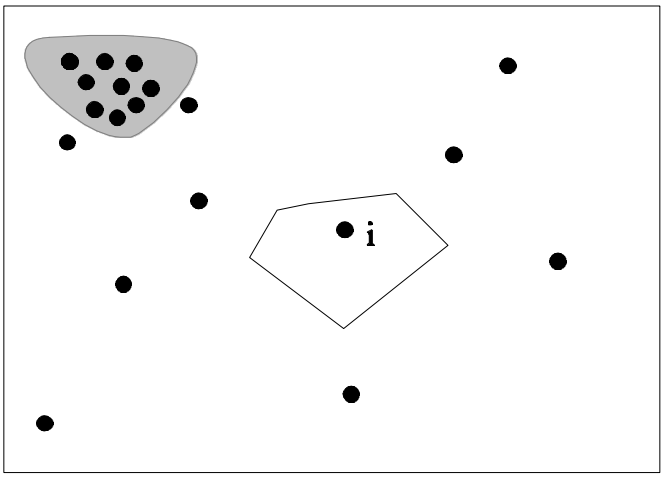

Figure G.14. The *polygon of influence* for point *i* (enclosed region)

In the polygonal method, a *polygon of influence* is constructed for each data point. A polygon of influence refers to the area around a data point for which all points are closer to that data point than any other. Figure G.14 demonstrates the polygon of influence for data point *i*.

The weight assigned to point *i* becomes the inverse area of the polygon of influence. This has the effect

of giving smaller weights to areas of dense sampling and more weight to sparser areas. This was similar to the section of the site in the previous analysis but is directed at single data points and is somewhat less arbitrary.

In cellular declustering, a grid is overlaid on top of the site (Figure G.15). The weight assigned to any data point is one over the number of data points occupying the same cell**.** This gives more weight to sparsely sampled areas as well.

Cell declustering has two particular disadvantages. First the weight assignment to any data point is not unique because one can specify different grid sizes. Second, if there is no underlying pseudo regular grid across the site, the approach tends to produce a poorer result than its polygonal counterpart (Isaaks and Srivastava 1989).

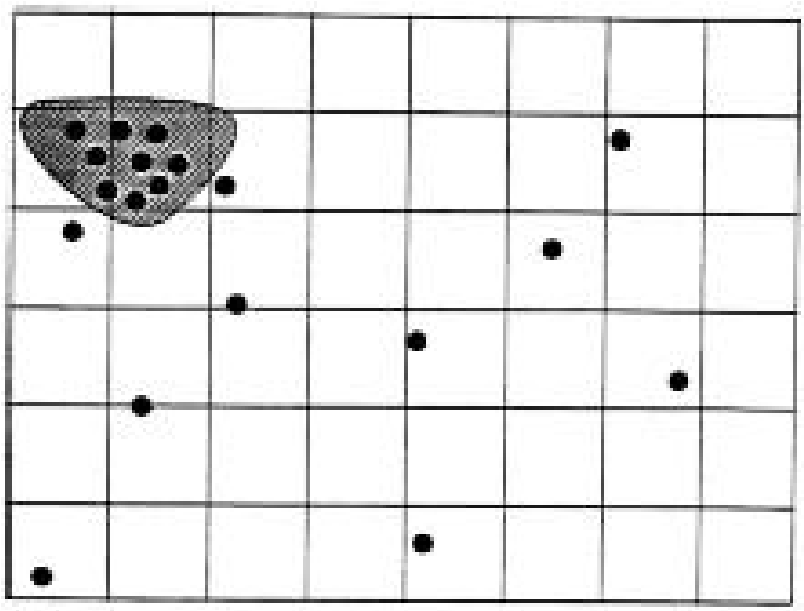

Figure G.15. Cellular declustering

The formulas for the sample mean, $\bar{x}$, and variance, s^2, of weighted data follow. These formulas assume that the sum of weights is one, i.e., $\sum_i^n w_i = 1.$. This can be achieved in each of the methods previously discussed by dividing individual weights $\sum_i^n w_i$.

$$\bar{x} = \sum_i^n w_i x_i \qquad s^2 = \sum_i^n w_i (x_i - \bar{x})^2$$

Confidence limits are constructed as before, $\bar{x} \pm 1.96\, s/\sqrt{n}$.

The sampled data set was declustered using cellular declustering with cells of length 13.4 and height 25. These where chosen because they where approximately the size of the two clustered areas. The mean and associated confidence intervals now are 198 < 214 < 231 pCi/g. Once again the interval contains the true mean of 216 pCi/g.

Declustering has made a significant improvement in the estimation of the mean over the clustered estimation. Other declustering algorithms are also available that might improve upon this estimate. In reality, it is impossible to know the degree to which one has improved an estimate and therefore difficult to compare declustering methods in practice. Two problems still remain with this analysis:

1. The assumption of normality is not supported by the raw data.

2. The fact that the data are spatially correlated has not been statistically recognized. This can have produce confidence limits that are too small.

G.3.5 Spatial Correlation

Contamination occurs across space as the result of a physical phenomena. As a result, sample data are usually spatially correlated. For example, data sampled close together are more likely to be the same than data sampled far apart. In other situations, data sampled in the same direction as in the cross section of a plume can be more alike than points sampled in the direction of the plume. Ignoring spatial correlation in calculation of exposure concentrations can be hazardous. In particular the calculation of confidence limits is adversely affected. Ignoring the presence of significant spatial correlation has the effect of severely underestimating confidence limits. This can be a serious error when using upper confidence limits as clean-up criteria.

A popular tool for measuring spatial variability[2] is the variogram denoted $\gamma(h)$. The variography consists of identifying all data points that are a certain distance apart and at a certain angle and calculating the variance of that set.[3] This is done incrementally for each distance to produce an experimental variogram that is typically fit with an analytical model. Figure G.16 shows an example of a modeled experimental variogram, which provides a visual description of how variability changes with distance.

In constructing confidence limits, spatial correlation is often described by the covariance $C(Z(s(i)),Z(s(j))) = C(h)$ where $h = |s(i) - s(j)|$, and s(i), s(j) are data sample locations. The covariance is related to the variogram:

$$C(h) = C(0) - \gamma(h) = \sigma^2 - \gamma(h).$$

A more general form for the variance on the mean $\sigma^2(\bar{x})$ is written as :

$$\sigma^2(\bar{x}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j cov(Z(s(i)),Z(s(j)))$$

and is typically larger than σ^2/n (Cressie 1993).

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[2] Consider variability to be the opposite of correlation.

[3] This method assumes that the variability of data depends only on their separation distance and not on their location.

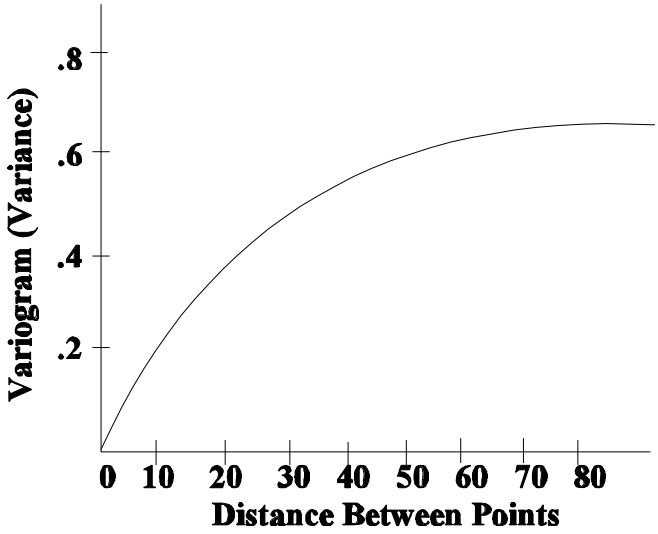

Figure G.16. Variography of the example data

In the case of the example data set, the data have already been declustered and will now be considered in light of the correlation structure. Applying the general form gives 176 < 214 < 253 as the confidence interval on the mean. Note that this interval includes the true mean of 216. In comparison, failing to recognize spatial correlation produces a calculated confidence interval of (198 < 214< 231 pCi/g) that would be reported as a 95% confidence interval. In reality the confidence level is only 60% since $1.96\sqrt{\sigma^2/n} = 0.85\sqrt{\sigma^2(\bar{x})}$. This effect becomes more pronounced as the correlation among data increases. An example of increasing correlation for the sampling design in the example problem corresponds to an increase in correlation length. As correlation increases spatially, data that are farther away are more alike and provide less information.

G.3.6 Dependence, Independence, and Equivalent Data

Data samples that are correlated have some degree of statistical repetition to them. For example sampling numerous times in the same spot produces little information from a statistical standpoint. Another way to quantify this effect is with the idea of *equivalent number of independent observations* (Cressie 1993). That is one can compute the relative efficiency of correlated observations with respect to their independent data counterpart. For example, the variance of the mean for independent data is given as σ^2/n. Denote the variance for the mean of dependent data as σ^2_D, which now is written as :

$$\sigma^2_D = \sigma^2/n' \ ,$$

where n' is interpreted as the equivalent number of independent observations. Solving for n' gives $n' = \sigma^2/\sigma^2_D$. In the example, $\sigma_D{}^2$ and σ^2 were estimated as 384 pCi/g and 6072 pCi/g, respectively. The effective number of independent observations is only 16 for this example. While in reality there are no independent observations available, this result demonstrates the significance of spatial correlation and the impact on the statistical analysis.

The following table compares the means and confidence limits for each level of analysis (pCi/g). Compare these to the true mean of 216 pCi/g.

Type of Analysis	Lower 95%	Mean	Upper 95%
Classical	265	282	300
Bonferroni	188	212	236
Declustered Data	198	214	231
Declustered and Spatial Correlation	176	214	253

G.3.7 Geostatistical Approach

The following estimates of exposure concentration all summarize the data with a single statistic and quantify the uncertainty about that statistic with a confidence interval. Other methods of data analysis exist that are designed to approximate concentration values at unsampled points to create a continuous image of contaminant concentration. These "interpolatory" approaches to data analysis can be either deterministic or stochastic models of contamination. Deterministic methods are not set in a probabilistic frameworks and the notion of mean, variance, and distribution are not usually part of the analysis. Examples include triangulation, inverse distance, and polynomial interpolation. In recent years, stochastic or probabilistic models of spatial estimation have gained popularity due to their flexibility and attention to statistical parameters seen in the data. A large family of stochastic estimators known as *the kriging* methods have demonstrated good results in many earth science applications. Kriging estimates the unknown concentration at an unsampled point by weighted values of nearby data. This is similar to the deterministic method of inverse distance. The difference lies in the formulation of the kriging weights which depend on a stochastic model with a measure of spatial covariance such as a variogram. Various forms such as ordinary and indicator kriging are well described in the literature (Isaaks and Srivastava 1989).

At this point an easy transition from the assumption of normality can be made.[4] A nonparametric form of kriging known as *indicator* kriging will be used here. The variogram structure observed in the declustered data was used to create an indicator kriging map of the example contamination (Figure G.17).

[4] Non-parameteric test are also available for analysis similar to those in the previous sections.

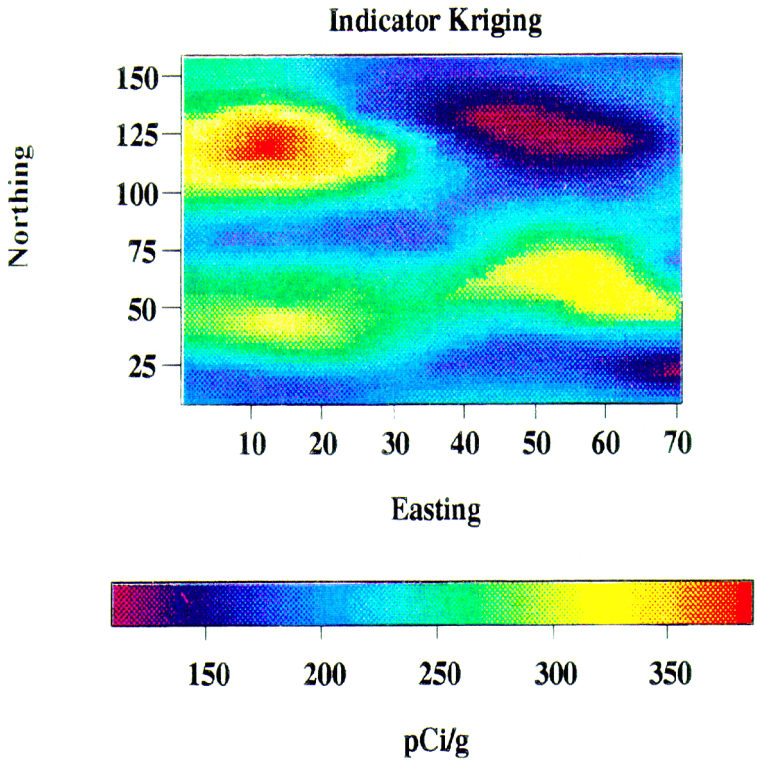

Figure G.17. Kriged map of contaminant concentrations

The power of kriging in estimating concentration levels lies in the ability to estimate concentration levels over areas of the site that would have had an insufficient amount of data otherwise. This is important in the case where the exposure unit is smaller than the area of contamination. It may be important to estimate the concentration over a subset of the site that has an insufficient amount of data. Kriging estimates concentration values at missing points within that area using data from across the site. This provides enough data to calculate an arithmetic mean and an estimate of the variance[5] and provides the tool for calculating concentration values for the scenario where units are smaller than the site.

A common complaint with kriged maps is that they are typically too smooth and the estimation lacks the variability seen in the data. As a result, the role of kriging has shifted from a primary mapper to a tool in the process known as *geostatistical* simulation. Instead of producing a single image of contamination across the site that is "best" in some statistical sense, simulation produces multiple and equiprobable estimations of contamination that can honor both the sampled data at their original locations as well as important statistics of the data set such as mean, distribution, and covariance structure. A compilation of these images provides a measure of joint uncertainty that is not possible through typical kriging applications (Deutsch and Journel

[5] The derivation of the method for calculating variance of kriged results is different and can be found described in detail in (Isaaks and Srivastava 1989)

1992).

By creating a continuous image of contamination and simultaneous and continuous uncertainty about the image, this allows one to estimate either the global mean or statistics about any subsection of the site. This is important particularly in the case where the exposure unit is smaller than the range of contamination. In those types of cases, it is not uncommon to have an insufficient amount of data to adequately estimate local statistics. Simulation provides the tools to fulfill these exposure unit requirements.

Two examples of simulation are the sequential gaussian and sequential indicator simulation routines. The first method assumes a multivariate normal distribution of the data values and implements ordinary or simple kriging as the estimator. Since a large body of earth science data can be modeled as a normal distribution, this is a highly popular form of simulation. It is well understood and has a successful track record. Indicator simulation provides a non-parameteric approach to simulation that is based on indicator kriging (Deutsch and Journel 1992).

The data in the example give little justification for assuming a normal distribution, so the indicator approach will be used. The declustered data as well as the necessary covariance structures[6] are determined, and 30 simulations are run. Figure G.18 shows two of the resulting simulations, and Figure G.19 shows the average of all thirty. With these thirty simulations, many powerful statistics and measures of uncertainty are possible.

Simulation provides an entirely separate decision rule for defining concentration terms. For example, over any given area, one may define the concentration term as:

- the maximum simulated value or data observed,
- the 95th percentile of all simulated values,
- the observed upper 95 percentile of observed simulation averages, and
- the average of observed simulation upper 95 percentiles.

For a more in-depth discussion of the use of geostatistics in environmental remediation, refer to *Geostatistical Applications in Environmental Remediation* (Stewart et al. 1995).

[6] For a complete description of the variography requirements of indicator kriging or simulation see (Deutsch and Journel 1992).

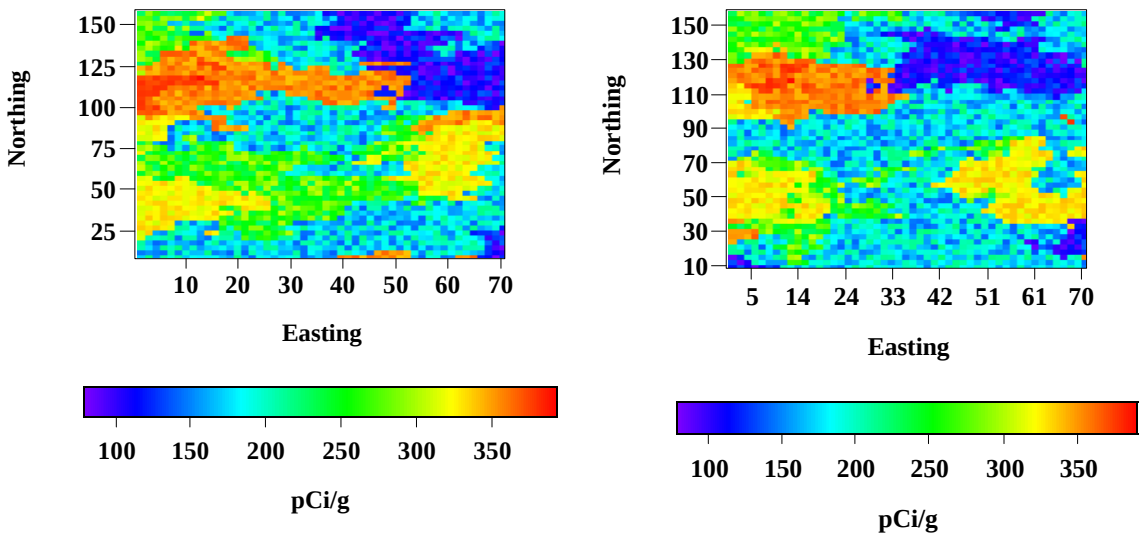

Figure G.18 Two simulation results.

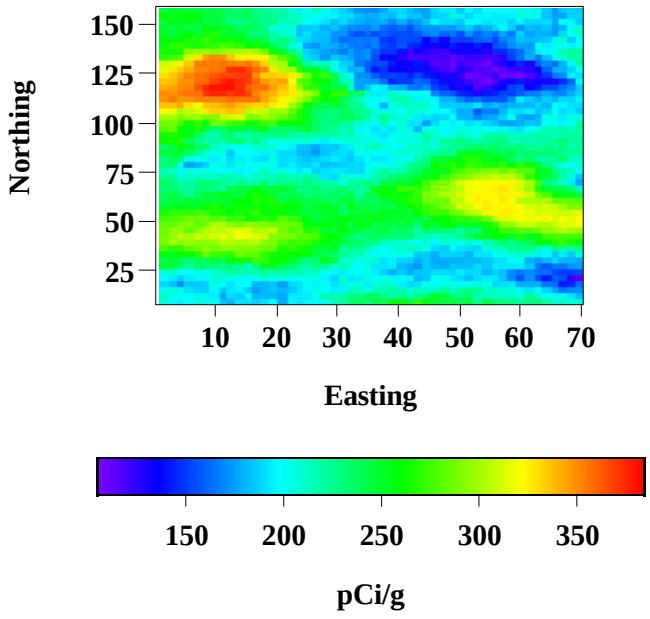

Figure G.19. Average of 30 simulations

G.3.8 Recommendations

Several methods of dealing with environmental data for the purposes of risk assessment exposure calculations are given to demonstrate the effects of deviations from basic assumptions and the failure to incorporate valuable spatial information. For the methods presented in this white paper, an increase in the complexity of the analysis increases the number of data required to support the analysis. The degree to which the data support the analysis must be decided on a site-specific basis. In lieu of site-specific conditions, the following list presents the previous methods in order of their general increase in data requirements. It is recommended to use the highest level of analysis supported by the data.

1. Traditional approach
2. Bonferroni/declustering methods
3. Declustering and spatial analysis
4. Full geostatistical analysis (kriging and simulation)

For practical purposes, it is recommended that geostatistical analysis be used while incorporating all the available or pertinent data to estimate concentrations in subset areas where an insufficient amount of sampling data are available.

G.4. DEALING WITH CENSORED DATA

A detection limit (DL) is a measurement value below (or above) which accurately reported concentration values are not determinable. The DL is not truly an absolute number but rather a statistically derived value. In particular, the DL is the lowest measured value that can be shown to be statistically different from zero (Berthouex 1993). This requires the calculation of measurement errors typically estimated by measuring reference materials of known concentration (including blanks of zero concentration).

Data that fall below this limit are reported in several ways: (1) trace, (2) "ND" for not detected, (3) the DL itself, (4) < DL, (5) zero, (6) a value between zero and DL, and (7) actual concentration with a measure of accuracy as $x \pm e\ pCi$. These data are said to be *left censored*. For studies with upper detection limits, the data are said to be *right censored*. The latter is more common in survival analysis and is not commonly encountered in exposure assessment. When discussing DLs, this white paper will refer to left censored data.

The issue of censored data in a statistical analysis is important especially for low level exposure limits. The method chosen to deal with nondetects can significantly impact an analysis affecting statistical moments such as the mean and standard deviation. In risk assessment, where values used to estimate lifetime risk accumulate, the left censored data can become very important (Perkins et al. 1990). The issue is further complicated in a geostatistical analysis by the inclusion of a spatial component in determining concentrations. This white paper considers three common ways of dealing with censored data, which are among the most practical to implement, along with a discussion of their limitations.

G.4.1 Values Between Zero and the Detection Limit (DL)

In practice, it is common to assign a value of DL or DL/2 to all values less than DL. The assumption for the latter is that, on average, censored data are about half the detection limit; this assumption can generate a great deal of error depending on the size and shape of the distribution (Perkins et al. 1990). Kushner (1976)

concluded that the DL/2 method was appropriate if there is reason to believe that data below DL were uniformly distributed or if it could be established that the error in this assumption would be insignificant in the presence of error due to a finite sample and measurement noise. If data are lognormal, the error in using the DL/2 could be significant. In Kushner's example, the geometric standard deviation and geometric mean where underestimated by as much as 20% depending on the percentage of censored data.

G.4.2 Fill-in Methods

"Fill in" methods assume that the data follow a given distribution. In this approach, it is assumed that the left tail of the distribution is missing due to the DL. This tail is filled in by replacing below DL data with realizations randomly drawn from a distribution model that fits the uncensored data via a predefined criterion. For example, if the data are normally distributed, the mean and standard deviations of the uncensored data are calculated and used as parameters in the normal random variable model of the data. If there are *n* censored samples, then *n* realizations are drawn from the normal distribution on the interval (0, DL). This complete data set is then used in further statistical analysis; this procedure is similar for the lognormal model.

An alternative formulation of the fill-in method stems from the argument that information about the DL could be better incorporated by including some fraction of DL in the initial calculation of the mean and standard deviation. Gilliom and Helsel (1986) make an initial use of the censored data by substituting half the DL for each censored sample in the calculation of mean and standard deviation. Once the model is constructed, the censored data are replaced by realizations drawn from below the DL, and the mean and variance are recomputed. Haas and Scheff (1990) argue that this is not a unique solution. Clearly, one could choose any initial substitution value and obtain a different overall distribution. Glelt (1985) uses an iterative process by substituting the expected value of the normal order statistics for the censored samples. At each iteration, the mean and variance are calculated using the expected value for data less than the DL as the replacement value of the censored data. This is repeated until there is a negligible change in the mean and variance.

Another fill-in technique assumes that everything below the DL should be modeled as a uniform distribution on the interval [MIN, DL] where MIN is the lowest possible measurement In this method, the uncensored data provide no information about the left hand tail. Nehls and Akland (1973) argue that, in the vicinity of the detection limit, data appear to be distributed as a random variable; however, Kushner (1976) points out that Nehls and Akland provide no data to support this claim nor do they suggest where the uniform distribution ends and the normal begins. Despite these arguments, uniform fill-in may be the model of choice where a large percentage of the data is censored or inadequate for estimating parameters for normal or lognormal distributions. Cohen and Ryan (1989) use this method when more than 50% of data are below DL.

G.4.3 Extrapolation Methods

In a similar approach to the fill-in method, extrapolation methods make assumptions about the censored tail from the noncensored data. For data modeled as normal or lognormal, data are plotted respectively on a normal or log probability scale. If there are n' missing data out of *n* available, then the first uncensored data (ordering from smallest to largest) are plotted as $x_{n'+1}$ versus the $[(n'+1) - .5]100/n$ percentile (Gilbert 1987). On these scales, the data form a straight line that can be fit with a least squares regression line; this line is then extended into the left censored region to provide an extrapolated estimation of the censored data. The mean and standard deviation for either distribution can be estimated from the probability plots. The mean and standard deviation for lognormal data are given by Gilbert (1987) where:

$$\mu = \exp(\hat{\mu} + \sigma^2/2)$$

$$\sigma = \mu[\exp(\hat{\sigma}^2 - 1)]^{1/2}$$

$$\hat{\mu} = \ln x_{0.50}$$

$$\hat{\sigma}^2 = \left\{ \ln \left[\frac{1}{2} \left(\frac{x_{0.50}}{x_{0.16}} + \frac{x_{0.84}}{x_{0.50}} \right) \right] \right\}^2 .$$

The mean and standard deviation for normal data are given by:

$$\mu = x_{0.50}$$

$$\sigma = \frac{(x_{0.84} - x_{0.16})}{2} .$$

Other methods include maximum likelihood techniques and product limit estimations. These techniques and others are too extensive to discuss here and can be found in the available literature (Gilbert 1987; Kushner 1976; Perkins et al. 1990; Gunter 1994).

As a balance between practical applications and performance, it is recommended that the extrapolation methods be used when possible. Substituting simple values below detection limits may be required when a large percentage of the data are censored.

G.5 GEOSTATISTICS AND THE EXPOSURE UNIT

Section G.2 presented solutions or guidelines to determining exposure unit size that are independent of the particular data at hand. These suggestions were motivated by the need to define pathways that are realistically possible and more closely related to actual pathways scales observed from available data. Clearly, there are at least two limitations with the guidelines presented. In some cases, they may present a less than satisfactorily conservative estimate of concentration. Second, they require a clear definition of the spatial extent of contamination. A conservative estimate and a clear definition of the extent of contamination are needed to appropriately place the exposure unit and identify whether multiple units could fit within the contaminated area. If one wishes to use the entire site as an exposure unit (for small sites) or if one wishes to more closely examine the spatial distribution of contamination to better assess the question of multiple units, the geostatistical analysis presented in Sect. G.3 presents a powerful tool in quantifying the state of knowledge about contaminant dispersion.

With only the sample data, several methods of subdividing the data into exposure units are possible. Each of these can produce a different concentration term within an exposure unit as demonstrated in Sect. G.2. Currently, each of these are equally likely, leading to conflict about the best choice.

The simulation presented in Sect. G.3 is a powerful tool to this effect, and the most typical application of simulation or kriging is to define the spatial extent of contamination. Several benefits of the procedure exist, including:

- a defensible approach to modeling spatial dispersion of contamination [geostatistics has already had a successful track record in environmental litigations (Stewart et al 1995)],
- an estimate of the "boundary" of contamination for any given contaminant threshold,
- assistance in defining the logical aggregation of data within a site which will define operable units,
- an estimate, for a given boundary, of the percentage of contaminated media that will be incorrectly classified as clean (Type I error), and
- an estimate of the percentage of clean media that will be incorrectly classifed as contaminated (Type II error).

The simulation output already presented in Sect. G.3 can be used to simulate these principles. Figure G.20 presents an average of point simulations over the entire site.

Suppose that one wanted to define the contamination at levels above 300 pCi/g. The geostatistical simulations model the spatial point averages shown in Figure G.21 as exceeding 300 pCi/g.

If one defines these areas to be the exposure unit, then the simulations predict that approximately 16% of the soil will be misclassified as being clean (Type I error). That is, about 16% of the site could still exceed 300. Similarly, approximately 1.4% of the soil will be misclassified as being contaminated (Type II error). These misclassifications arise from the spatial uncertainty about contamination. Typically, the Type I errors as defined here are the most serious errors. The Type II errors are significantly smaller in this example. The reason for this is that those areas of high contamination (above 300 pCi/g) are highly characterized, and the simulations are invariant. In contrast, those areas around the hotspots are not nearly as well characterized; therefore, the simulations are more variable in classifying the contamination as above 300 pCi/g.

This ability to quantify uncertainty is a powerful feature of a geostatistical model. It permits one to shift the point of decision from a qualified guess about contaminant dispersion to a decision about acceptable risk of a Type I error. For example, if one defines the clean-up limit to be 300 pCi/g and is willing to accept a 20% chance of misclassifying any point, then the boundaries of contamination are shown in Figure G.22. In fact, for any contamination level, a probability map can be drawn to demonstrate the probability of misclassification (Figure G.23).

Given a boundary, one can estimate the volume of misclassified media by observing predicted contamination across the boundary for each simulation. For example, the boundary established by the 20% risk level can expect to misclassify about 5% of the site as clean. This is an important link between pointwise risk and volume error. In Figure G.23, the estimated Type I and II volumes for each pointwise level of risk is computed. As the tolerance for pointwise Type I decreases so does the Type I volume. The tradeoff is that the Type II volume increases so that large volumes are being classified as contaminated when they are not contaminated; this misclassification ultimately can be very costly in clean-up efforts. Decision makers must decide which error they are more willing to make.

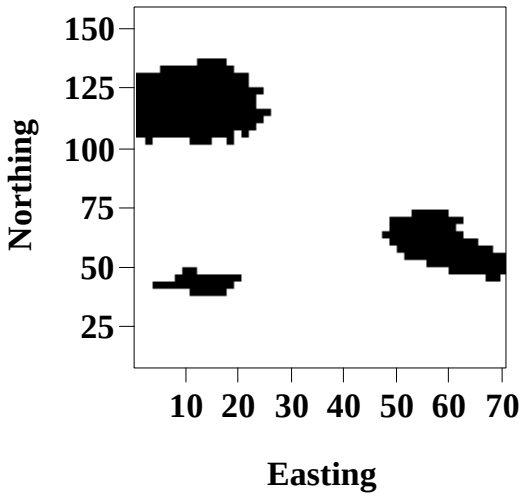

Figure G.20. Areas where simulation averages exceed 300

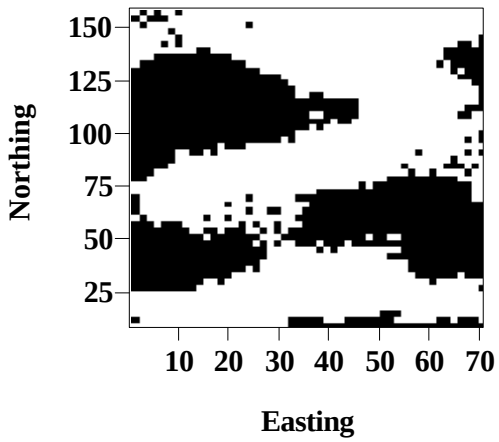

Figure G.21. Areas where chance of exceeding 300 pCi/g exceeds 20%

By defining contamination boundaries based on the data, another logical, technically defensible method for the aggregation of data in defining operable units is available. Once a unit has been defined, one can use the original data that fall within these areas or may use the estimated values to estimate the mean and variance[7]. When possible, one could use both methods of defining exposure units to arrive at better exposure unit concentrations. One could use the geostatistics to define the extent of contamination and use the methods previously described to define units within those contamination boundaries.

G.6. CONCLUSION

This white paper presents several methods for dealing with problems of preferential sampling, sample correlation, and deviations from normality as well as recommendations on defining exposure unit sizes are presented. A fundamental issue that is prevalent throughout the paper is the influence of spatial factors. These influences must be considered when deriving a reasonable, technically defensible estimate of the concentration. Exposure unit size recommendations are given but should be used along with site specific conditions to arrive at the best solution for the particular site. The analytical methods presented for dealing with exposure concentration calculations should improve concentration estimation for a large class of problems. Other methods are available and are mentioned in the text as well. The level of analysis that can be supported is dependent on the amount and quality of the data available. If there are little data, then neither traditional nor geostatistical approaches likely will be adequate. One must decide when a given level of analysis can be technically defended. This is a site-specific factor and must be dealt with by statisticians and risk assessors on a site-by-site basis.

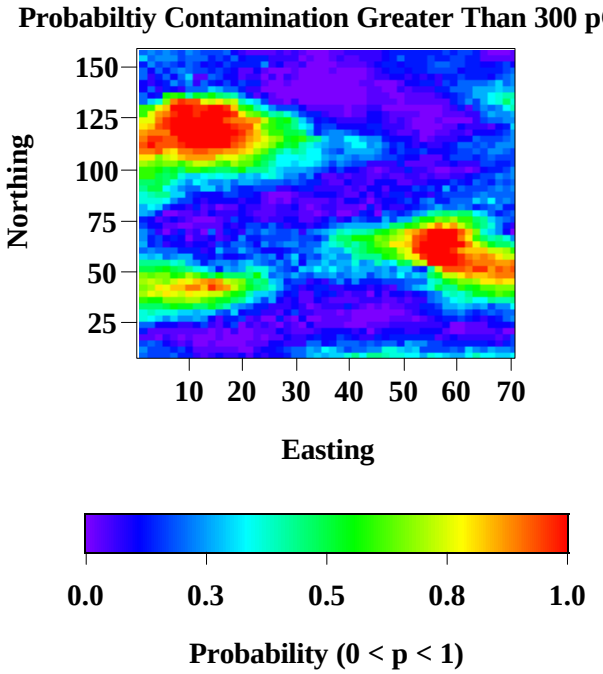

Figure G.22. Probability of exceeding 300 pCi/g at each point

[7] See Isaaks and Srivastava (1989) for a discussion of estimation variance.

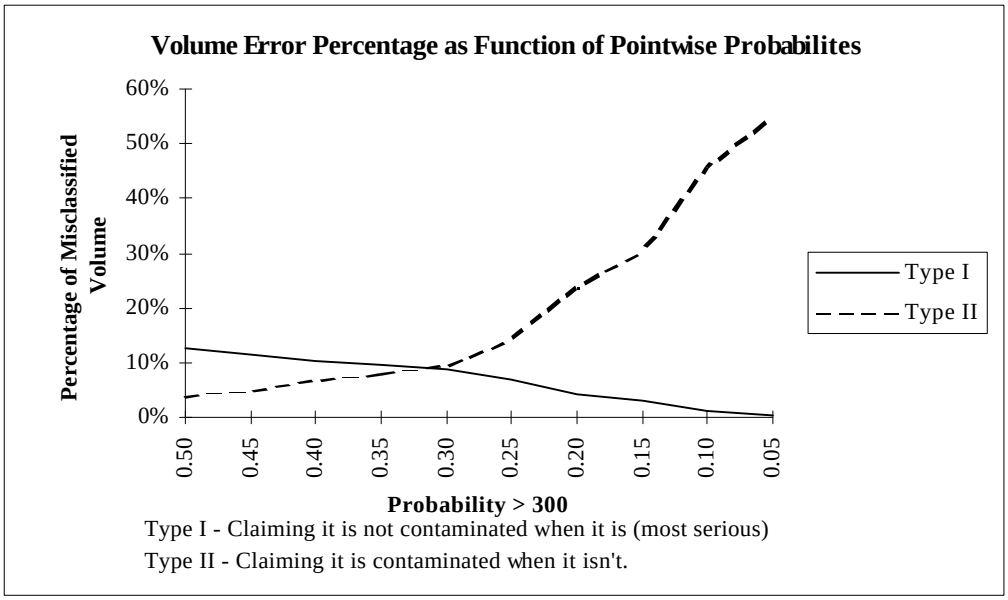

Figure G.23. Relationship between Type I and Type II errors for the example problem

G.7. REFERENCES

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APPENDIX H

UNCERTAINTIES ASSOCIATED WITH RESIDENTIAL RISK PATHWAY MODELS FOR SOIL AND GROUNDWATER

H.1. INTRODUCTION

The quantitative assessment of uncertainties in the exposure parameters for the individual exposure pathways provides considerable information about the variability and sensitivity of the calculated results. These results are important because point estimates of these parameters are used to determine the extent of remediation necessary through the Superfund process. The point estimates that are provided as guidance by the U.S. Environmental Protection Agency (EPA) are often conservative and can result in an overestimate of the potential risk. The scope of this work is to perform an uncertainty analysis on the standard Superfund residential scenario risk equations using available statistical information for the uncertain exposure parameters. The results are used to quantify the degree to which the standard default values overestimate the predicted percentiles of exposure (90–95th) that they are intended to estimate and to determine which parameters are responsible for the majority of the variation.

Residential exposure pathways associated with contaminated soil and groundwater are evaluated in this report and include the ingestion, inhalation, and dermal contact pathways. The external exposure pathway from exposure to soil contaminated with radionuclides is also evaluated. Exposure calculations are performed using models present in the EPA's *Risk Assessment Guidance for Superfund*. In this document, these models are not used to calculate actual risk values. Instead, the exposure parameters generally held to be constant for all sites are used to evaluate the variability in the predictions of the individual models. Uncertainties in the risk estimates that result from site- or contaminant-specific variability are not assessed for this effort. For the exposure parameters, a sensitivity analysis is performed to determine the most sensitive parameters in each model.

The outcome of this work can be used to focus the attention of the risk assessor on the expected variability, range of variation, and therefore the reliability of the point estimates that are used, and on the parameters that caused the variation. In addition, a relative ratio between the point estimates (PE) as set forth in EPA guidance and the predicted percentile risk results is presented for each pathway analyzed. The predicted percentiles of the exposure parameters are referred to as multiplicative exposure factors (MEF). These PE/MEF ratios are used to quantify the degree of conservatism present in the default exposure parameters that are recommended by the EPA for Superfund sites for each residential pathway analyzed. This general method of determining a multiplicative exposure factor that is constant for all sites can be used to derive values for the exposure term that are more representative of the EPA's stated risk management goal of protecting 90 to 95% of the potentially exposed population for a given land use scenario. Alternatively, these ratios can be used as part of the uncertainty assessment in a baseline risk assessment to estimate the degree of conservatism present in the exposure parameters of each pathway.

The probabilistic distributions of the uncertain exposure parameters used in these models are collected from the most recent sources in the literature. The parameters for which distributions are assigned include exposure frequency, exposure duration, body weight, surface area to body weight, ingestion rates for water and soil, inhalation rate, exposure fraction, adherence of soil-to-skin factor, and the gamma shielding factor. Professional judgment is used to supplement the data and provide a distribution for the few parameters for which no consensus distribution is available.

H.2. RESIDENTIAL LAND USE RISK EQUATIONS

This section provides the equations and recommended point estimates provided in various EPA sources for the residential pathway. Under residential land use, residents are expected to be in frequent, repeated contact with contaminated media. For carcinogens, the exposure assumptions account for daily exposure over long term

and generally result in high potential exposures and risk. For noncarcinogens, the exposure assumptions do not account for accumulations over the life time of the exposed receptor. Risk from groundwater contaminants is assumed to be primarily from direct ingestion, inhalation of volatiles from household water use, and dermal contact while showering. Risk from soil is assumed to be from direct ingestion, inhalation of dust and particulates, dermal exposure from chemicals, and external exposure from radionuclides.

H.2.1 Groundwater Equations

H.2.1.1 Nonradionuclide Contaminant

For carcinogens, the exposure assumptions are considered in the long term; therefore, the uncertainty of the exposure duration will impact the model predictions. For noncarcinogens, the exposure assumption of a one time dose will nullify the effect of variation in the exposure duration. Mathematically, this is done by introducing the exposure duration as a factor of the averaging time in the denominator of the ingestion model.

1. Ingestion

$$Ingestion\ risk = C \times \left[\frac{IR_w \times EF \times ED}{BW \times AT}\right] \times TV_o \quad (1)$$

2. Inhalation of vapor-phase chemicals

$$Inhalation\ risk = C \times K \times \left[\frac{IR_a \times EF \times ED}{BW \times AT}\right] \times TV_i \quad (2)$$

3. Dermal contact

$$Dermal\ contact\ risk = C \times K_p \times CF_1 \times \left[\frac{SA \times ET \times EF \times ED}{BW \times AT}\right] \times TV_d \quad (3)$$

where:

Parameters	Definition (units)	Default Value
AT	averaging time (yr × day/yr)	70 × 365 (carcinogen) EPA 1991a) ED × 365 (noncar.) (EPA 1991a)
BW	adult body weight (kg)	70 (EPA 1991a)
C	chemical PRG in water (mg/L)	)
CF_1	units conversion factor (L-m)/(cm-m^3)	10
ED	exposure duration (yr)	30 (EPA 1991a)
EF	exposure frequency (day/yr)	350 (EPA 1991a)
ET	exposure time (hr/day)	0.25 (EPA 1992)
IR_a	inhalation rate (m^3/day)	20 (EPA 1995)
IR_w	water ingestion rate (L/day)	2 (EPA 1991a)
K	volatilization factor of Andelman (1990) (L/m^3)	0.0005×10^3

		(Andelman 1990)
K_p	permeability constant (cm/hr)	chemical-specific
SA	adult total body surface area (m^2)	1.94 (EPA 1992)
TV_{ad}	absorbed toxicity value	SF_{ad} (carcinogen) $1/RfD_{ad}$ (noncarcinogen)
TV_i	inhalation toxicity value	SF_i (carcinogen) $1/RfD_i$ (noncarcinogen)
TV_o	oral toxicity value	SF_o (carcinogen) $1/RfD_o$ (noncarcinogen)

H.2.1.2 Radionuclide contaminants

Since most radionuclides are not volatile, the inhalation pathway is not usually considered for exposure through groundwater. The special case radionuclides (e.g., tritium and radon) are not discussed in this document. Therefore, the only pathway that will be evaluated for groundwater in this study is the ingestion pathway:

$$Ingestion\ risk = C \times [\ IR_w \times EF \times ED\ ] \times SF_o \qquad (4)$$

where:

Parameters	Definition (units)	Default Value
C	radionuclide PRG in water (pCi/L)	)
ED	exposure duration (yr)	30 (EPA 1991a)
EF	exposure frequency (day/yr)	350 (EPA 1991a)
IR_w	water ingestion rate (L/day)	2 (EPA 1991a)
SF_o	oral slope factor (risk/pCi)	rad-specific (ORNL 1994)

H.2.2 Soil Equations

Under residential land use, risk of contamination from soil is caused by direct ingestion, inhalation of dust and particulates, dermal exposure to chemicals, and external exposure to radionuclides. Because the soil ingestion rate is different for children and adults, the carcinogenic risk due to direct ingestion of soil is calculated using an age-adjusted ingestion factor. This takes into account the differences in daily soil ingestion rates, body weights, exposure fraction, and exposure durations for the two exposure groups. Exposure frequency is assumed to be the same for the two groups. Calculated in this manner, the factor leads to a more protective risk-based concentration compared to an adult-only assumption. Due to differences in averaging times for carcinogens and noncarcinogens, the noncarcinogenic hazard is calculated separately for adults and children. This procedure will give a more protective concentration than the adult-only assumption.

H.2.2.1 Nonradionuclide contaminant

1. Ingestion

a. Carcinogen

$$Ingestion\ risk = C \times \times CF \times \left| EF \times \left(\frac{IR_c \times ED_c}{BW_c} + \frac{IR_a \times ED_a}{BW_a} \right) \times FI \right| \times \frac{TV_o}{AT} \quad (5)$$

b. Noncarcinogenic (adult and child calculated separately)

$$Ingestion\ risk = C \times CF \times \left[\frac{EF \times ED_n \times IR_n \times FI}{BW_n \times AT_n} \right] \times TV_o \quad (6)$$

2. Inhalation only

$$Inhalation\ risk = C \times \left[\frac{EF \times ED \times IR_{air}}{BW \times AT} \right] \times \left(\frac{1}{VF} + \frac{1}{PEF} \right) \times TV_i \quad (7)$$

3. Dermal contact only

$$Dermal\ contact\ risk = C \times CF_d \times ABS \times \left[\frac{SA \times AF \times EF \times ED}{BW \times AT} \right] \times TV_{ad} \quad (8)$$

where:

Parameters	Definition (units)	Default Value
ABS	absorption factor (unitless)	0.01 (organic) (EPA 1995) 0.001 (inorganic) (EPA 1995)
AF	adherence factor (mg/cm^2)	1 [11]
AT	averaging time (yr × day/yr)	70 × 365 (carcinogen) (EPA 1991a) ED × 365 (noncarc.) (EPA 1991a)
AT_n	averaging time - noncarcinogenic ingestion only (yr × day/yr)	ED_n × 365 (EPA 1991a)
BW	adult body weight (kg)	70 (EPA 1991a)
BW_n	body weight - noncarcinogenic ingestion only (kg)	70 (adult) (EPA 1991a) 15 (child) (EPA 1991a)
C	chemical PRG in soil (mg/kg)	)
CF	units conversion factor (kg/mg)	10^{-6}
CF_d	units conversion factor - dermal (kg-cm^2)/(mg-m^2)	0.01
ED	exposure duration (yr)	30 (EPA 1991a)
ED_n	exposure duration - noncarcinogenic ingestion	24 (adult) (EPA 1991a)

	only (yr)	6 (child) (EPA 1991a)
EF	exposure frequency (day/yr)	350 (EPA 1991a)
FI	fraction ingested (unitless)	1 [12]
IR_a	soil ingestion rate for adult (mg/day)	100 (EPA 1991a)
IR_{air}	total inhalation rate (m^3/day)	20 (EPA 1991b)
IR_n	soil ingestion rate - noncarcinogenic (mg/day)	100 (adult) (EPA 1991a) 200 (child) (EPA 1991a)
PEF	particulate emission factor (m^3/kg)	4.28×10^9 (see Eq. 40) (EPA 1991c)
RfD_{ad}	absorbed chronic reference dose (mg/kg-day)	chemical-specific (ORNL 1994)
RfD_i	inhalation chronic reference dose (mg/kg-day)	chemical-specific (ORNL 1994)
RfD_o	oral chronic reference dose (mg/kg-day)	chemical-specific (ORNL 1994)
SA	adult surface area (head, hands, forearms, lower legs) (m^2/day)	0.53 (EPA 1992)
SF_{ad}	absorbed dose slope factor ((mg/kg-day)$^{-1}$)	chemical-specific (ORNL 1994)
SF_i	inhalation slope factor ((mg/kg-day)$^{-1}$)	chemical-specific (ORNL 1994)
SF_o	oral slope factor ((mg/kg-day)$^{-1}$)	chemical-specific (ORNL 1994)
TV_{ad}	absorbed toxicity value	SF_{ad} (carcinogen) $1/RfD_{ad}$ (noncarcinogen)
TV_i	inhalation toxicity value	SF_i (carcinogen) $1/RfD_i$ (noncarcinogen)
TV_o	oral toxicity value	SF_o (carcinogen) $1/RfD_o$ (noncarcinogen)
VF	volatilization factor (volatile organics only) (m^3/kg)	chemical-specific (see Eqs. 34-39) (EPA 1991c)
W_c	average body weight from ages 1-6 (kg)	15 (EPA 1991a)
BW_a	average body weight from ages 7-31 (kg)	70 (EPA 1991a)
ED_c	exposure duration during ages 1-6 (yr)	6 (EPA 1991a)
ED_a	exposure duration during ages 7-31 (yr)	24 (EPA 1991a)
IR_c	ingestion rate of soil ages 1 to 6 (mg/day)	200 (EPA 1991a)
IR_a	ingestion rate of soil ages 7 to 31 (mg/day)	100 (EPA 1991a)

H.2.2.2 Radionuclide contaminant

1. Ingestion

$$Ingestion\ risk = C \times CF \times [\ EF \times (IR_c \times ED_c + IR_a \times ED_a) \times FI\ ] \times SF_o \quad (9)$$

2. External radiation only

$$External\ risk = C \times T_e \times [\ ED \times EF_x \times (1 - S_e)\ ] \times SF_x \quad (10)$$

where:

Parameters	Definition (units)	Default Value
C	radionuclide PRG in soil (pCi/g)	)
CF	units conversion factor (g/mg)	10^{-3}
ED	exposure duration (yr)	30 (EPA 1991a)
EF	exposure frequency (day/yr)	350 (EPA 1991a)
EF_x	exposure frequency - external (day/day)	350/365 (EPA 1991a)
FI	fraction ingested (unitless)	1 [12]
IR_a	soil ingestion rate for adult (mg/day)	100 (EPA 1991a)
S_e	gamma shielding factor (unitless)	0.2 9EPA 1991a)
SF_o	oral slope factor (risk/pCi)	radionuclide-specific (ORNL 1994)
SF_x	external exposure slope factor ((risk-g)/(pCi-yr))	radionuclide-specific (ORNL 1994)
T_e	gamma exposure time factor (hr/hr)	24/24 (EPA 1991a)

H.3. UNCERTAIN PARAMETERS

For the groundwater equations (i.e., Eqs. 1 through 4), the assessed parameters are the ingestion rate, inhalation rate, exposure frequency, exposure duration, averaging time, body weight, surface area, and exposure time. For the soil equations (i.e., Eqs. 5 through 10), the assessed parameters are the ingestion rate, inhalation rate, exposure frequency, exposure duration, averaging time, body weight, surface area, adherence of soil-on-skin factor, and fraction ingested. Specific uncertain parameters were collected for two age groups (children and adults).

Table H.1 summarizes the varying parameters used in the groundwater and soil exposure pathway equations. Their statistical distribution, descriptive statistics, and source of information is also presented.

Table H.1. Uncertain parameters and corresponding statistical distributions used in the groundwater and soil models

Parameter	PE	Distribution	Mean	S.D.	Min.	Max.	Likeliest	Reference
EF(days/year)	350	Triangular			180	365	345	Smith 1994
ED_{adult} (year)	30	Lognormal	11.36	13.72				Israeli 1992
ED_{child} (year)	6	Lognormal	11.36 truncate at 6	13.72				Israeli 1992
BW_{adult}	70	Lognormal	77.1	13.5				Smith 1994
SABW(m^2/kg)	0.027	Normal	0.025	0.003				Finley 1994b
IR_{water}(L/day)	2	Lognormal	1.26	0.66				Smith 1994
IR_{air}(m^3/day)	20	Uniform			5.05	17.76		Finley 1994a
ET(h/day)	.25	Triangular			0.13	0.33	0.20	Smith 1994
IR_{child}(mg/day)	200	Triangular			5	500	100	Finley 1994b
IR_{adult}(mg/day)	100	Triangular			0.1	50	25	Lagoy 1987
FI_{child}	1	Uniform			0.1	1		Finley 1994a
FI_{adult}	1	Uniform			0.1	0.5		Finley 1994a
AF(mg/cm^3)	1	Lognormal	0.52	0.9				Finley 1994c
Se	0.2	Triangular			0.0	1.0	0.2	Judgement

The following subsection elaborates on these data and compares the ranges of variation of these parameters with the point estimates recommended by EPA guidance.

H.3.1 Ingestion Rate of Groundwater

EPA's recommended value for an adult's ingestion rate of water is 2 L/day. A lognormal distribution with a geometric mean and a geometric standard deviation of 0.11 and 0.49 (i.e., arithmetic values of 1.26 and 0.66 L/day), respectively, was used by Smith (1994) and is reproduced for this study.

H.3.2 Ingestion Rate of Soil

The ingestion rates of soil recommended by EPA are 100 and 200 mg/d for adults and children, respectively. Lagoy (1987) suggested an average ingestion rate of 25 mg/d for adults. Other studies indicate that a 50 mg/day is likely to be an overestimate. Therefore, soil ingestion was assigned a value of 25 mg/day as the most likely value in a triangular distribution with minimum and maximum values of 0.1 and 50 mg/d, respectively. Finley et al (1994b) suggested a uniform distribution between 5 and 50 mg/day for children. Based on several studies, Lagoy (1987) suggested 100 mg/day as the soil ingestion rate for an average child and a value of 500 mg/day for a maximally exposed child. For this study, these values were selected as the most likely and the maximum values in a triangular distribution with a minimum value of 5 mg/d.

H.33 Inhalation Rate

Finley et al. (1994b) used a uniform distribution with minimum and maximum values of 5.04 and 17.76 m^3/day, respectively, for the inhalation rates for adults. These values were reported by EPA (1989) and are

reproduced in this document.

H3.4 Exposure Frequency

This parameter estimates the number of days per year that an individual may be exposed to a contaminated source. For the residential scenario, EPA generally recommends an exposure frequency of 350 days/year. Smith (1994) suggested a triangular distribution with minimum, maximum, and most likely values of 180, 365, and 345, respectively.

H.3.5 Exposure Duration

For the residential scenario, EPA recommends a point estimate of 30 years. Based on housing surveys, statistical analysis, and modeling of the moving process, Israeli et al. (1992) found that the average total residence time (i.e., exposure duration) varies between different housing categories (Table H.2).

Table H.2. Values, standard errors and standard deviations of the average total residence time for each housing category, Israeli et al. (1992)

Housing category	Average residence time (years)	Standard deviation (years)
All households	4.55 ± 0.60	8.68
Renters	2.35 ± 0.14	4.02
Owners	11.36 ± 3.87	13.72
Farms	17.31 ± 13.81	18.69
Urban	4.19 ± 0.53	8.17
Rural	7.80 ± 1.17	11.28
Northeast region	7.37 ± 0.88	11.48
Midwest region	5.11 ± 0.68	9.37
South	3.96 ± 0.47	8.03
West	3.49 ± 0.57	6.84

For this study, a lognormal distribution of the residence time of owners values are selected to represent the statistical distribution of the exposure duration of a potential adult resident. The same distribution truncated at 6 years is used to represent children.

H.3.6 Body Weight

EPA's body weight recommended values are 70 and 15 kg for adults and children, respectively. For adults, a lognormal distribution with a geometric mean and a geometric standard deviation of 4.34 and 0.17 (i.e., arithmetic values of 77.1 and 13.5 Kg), respectively, were used by Smith (1994). For children, the same reference suggested a triangular distribution with 6.5, 26.1, and 15 as the minimum, maximum, and most likely

values. These values are used in this study.

H.3.7 Surface Area

EPA's recommended value for an average surface area of a male adult body is 1.94 m^2. Since surface area is a function of the body weight, Finley et al. (1994b) developed a relationship between skin surface area, body weight, and age based on lognormally distributed factors. These factors are presented in Table H.3.

Table H.3. Distribution factors for total skin surface area/body weight ratio by age

Age	Arithmetic mean (cm^2/kg)	Standard deviation (cm^2/kg)
0-2	641	114
2-18	423	76
>18	248	28

For the dermal contact pathway, the distribution factors of this ratio are used to account for the resultant variation of the surface area and the body weight for both children and adults.

H.3.8 Exposure Time

EPA's recommended value for average exposure time in the shower is a value of 12 min/day. Smith (1994) suggested a triangular with minimum, maximum, and most likely values of 8, 20, and 12, respectively.

H.3.9 Averaging Time

For carcinogens, the averaging time is constant with a value of 70 years; for noncarcinogens, the averaging time is a function of the exposure duration. Therefore, variation in the numerator (exposure duration) will be nullified by the equivalent variation in the denominator (averaging time).This is expected because exposure in this case is not an aggregate exposure over the life time of the exposed individual.

H.3.10 Fraction Ingested

EPA's recommended value for the fraction ingested for both children and adults is 1. Finley (1994a) suggested a uniform distribution with a range of 0.1 and 1 for children and 0.1 and 0.5 for adults. These values were used for this study.

H.3.11 Adherence of Soil-on-Skin Factor

EPA's rough estimates for average and upper-bound soil adherence factors are 0.2 and 1.0 mg/cm^2, respectively. Finley (1994c) developed a standard soil-on-skin adherence probability density function using Monte Carlo analysis based on all data collected for all age groups. The distribution is lognormal with an arithmetic mean of 0.52 mg/cm^2 and a standard deviation of 0.9 mg/cm^2.

H.3.12 Shielding Factor

EPA's recommended value for the shielding factor is 0.2. Based on professional judgment, a triangular

distribution was assigned for this parameter with minimum, maximum, and most likely values of 0, 0.2, and 1, respectively. The minimum and maximum values represent the possible range for the parameter.

H.4 UNCERTAINTY AND SENSITIVITY RESULTS

Uncertainties in the predictions of risk based on Eqs. 1–10 are evaluated by assessing the variability of the results associated with the uncertainties in the corresponding input parameters. Those parameters are square bracketed in Eqs. 1–10. Note that parameters outside the square brackets are either constants or treated as constants. Additionally, standard values were selected for chemical-specific parameters to pursue the calculations. Therefore, the risk estimates are not necessarily meaningful other than for the evaluation of the variability in the predictions of the individual models due to variations in the uncertain parameters. Further, the different predicted percentiles of the risk estimates were compared to the point estimate of each model to develop a relative risk ratio which can be used as tool to quantify the credibility and the conservatism of the point estimates.

Statistical analyses of the model predictions are presented in terms of the coefficient of variability (COV) and therefore the range of variation. The COV is the ratio of the standard deviation to the predicted mean value. Therefore, a higher COV indicates a wider range of variation in the multiplicative exposure factor. Correlations between parameters are not accounted for in this study. Inclusion of correlation would have the net effect of reducing the COV value.

The uncertainty analysis was performed using the software package Crystal Ball, Version 3.0 (Decisioneering, Inc. 1993). Crystal Ball performed Monte Carlo simulations, for the probabilistic distributions of the uncertain exposure parameters, using the Latin Hypercube Sampling technique to predict the multiplicative exposure factor distributions.

H.4.1 Groundwater Pathways

Table H.4 presents a descriptive statistical analysis of the Monte Carlo simulations of the risk predictions associated with uncertainties in the input parameters for the exposure models and for the point estimates of the multiplicative exposure factors.

Table H.4. Results of the uncertainty analysis for the groundwater exposure pathways

	Carcinogens			Noncarcinogens			Radionuclides
Statistics	Ingestion	Inhalation	Dermal	Ingestion	Inhalation	Dermal	Ingestion
COV	1.37	1.24	1.21	0.58	0.40	0.26	1.33
Minimum	4.9E-5	3.1E04	2.2E-4	1.8 E-3	1.6 E-2	1.9 E-2	8.1 E+1
50%	1.2E-3	6.0E-3	4.4E-3	1.2E-2	5.9E-2	4.4E-2	2.4E+3
95%	7.4E-3	3.3E-2	2.2E-2	2.9E-2	1.1E-1	6.6E-2	1.4E+4
97.5%	1.0E-2	4.4E-2	3.2E-2	3.4E-2	1.2E-1	7.1E-2	1.9E+4
Maximum	4.7 E-2	1.4E-1	9.9 E-2	6.6 E-2	1.7 E-1	8.8 E-2	7.3 E+4
Point Estimate (PE)	1.2E-2	5.9E-2	2.9E-2	2.7E-2	1.4E-1	6.6E-2	2.1E+4
PE/(95%)	1.6	1.8	1.3	0.9	1.3	1.0	1.5
PE/(97.5%)	1.1	1.4	0.9	0.8	1.2	0.9	1.1

This table shows that for both nonradioactive and radioactive carcinogens, the COVs are greater than 1, which implies multiple orders of magnitude of variation over the range of the model predictions. For noncarcinogens, the variability in the model predictions is much less.

The relative risk ratio (PE/MEF) is calculated to determine the location of the point estimates with respect to the uncertainty predictions of the individual models. The calculations of relative risk ratios, which is the ratio of the PE to the predicted percentiles, show that the PE lies in the last 5% predictions of the Monte Carlo simulations for all exposure pathways. The ratio varies between one and two for the different exposure pathways. For example, for the ingestion of groundwater pathway, the ratio of the PE to the 97.5% was 1.13, which means that the PE is almost equivalent to the 97.5 percentile prediction. This indicates that the EPA default parameters are reasonable approximations of the upper percentiles of the multiplicative exposure factors.

Table H.5 presents the corresponding sensitivity analysis of the risk predictions associated with uncertainties in the input parameters for all groundwater exposure factors. The sensitivity results are limited to those exceeding 1% contribution.

Table H.5. Results of the sensitivity analysis for the groundwater exposure pathways

	Carcinogens			Noncarcinogens			Radionuclides
Sensitivity data	Ingestion	Inhalation	Dermal	Ingestion	Inhalation	Dermal	Ingestion
ED	**77%**	**84%**	**92%**	.	.	.	**79%**
IR_w	**18%**	.	.	**83%**	.	.	**18%**
BW	3%	2%	.	**10%**	**14%**	.	.
EF	2%	2%	2%	6%	**12%**	**31%**	2%
SABW	.	.	1%	.	.	**15%**	.
ET	.	**11%**	4%	.	.	**53%**	.
IR_{air}	.	.	.	.	**74%**	.	.

This table shows that for both nonradioactive and radioactive carcinogens the most important parameter of those evaluated in the risk models is the exposure duration parameter. Therefore, significant reduction in the range of variation of the exposure results can only be accomplished by reducing the COV for this variable. However, this parameter reflects the expected variability in the amount of time people live in a residence and it is not expected that this uncertainty can be reduced through the collection of additional data. For noncarcinogens, where the exposure duration plays no role in the variations of the risk predictions, the variability in the model predictions are affected by several other parameters. Contributions of sensitive parameters exceeding 10% are bolded. The following subsections elaborate on the exposure results for each pathway of the carcinogenic, noncarcinogenic, and radioactive exposure models.

H.4.1.1 Exposure to nonradioactive carcinogens in groundwater

The COVs for ingestion, inhalation, and dermal contact pathways for groundwater are 1.37, 1.24 and 1.21, respectively. The variation in the model predictions are expected to be wide based on these COVs, and the predicted multiplicative exposure factors vary by two to three orders of magnitude from the predicted minimas.

For the ingestion pathway, sensitivity analysis shows that in addition to the exposure duration parameter (77%), the water ingestion rate parameter has an additional impact (18%) on the predicted variability. The body weight and the exposure frequency have insignificant contributions.

For the inhalation pathway, sensitivity analysis shows that the inhalation rate parameter follows the exposure duration (84%) with a very limited impact (11%) on the predicted risk. The body weight and the exposure frequency have insignificant contributions.

Sensitivity analysis for the dermal contact pathway shows that the variation in the risk prediction is 92% due to variation in the exposure duration over its distribution. Variation in the risk prediction due to variations in all other uncertain parameters is negligible.

H.4.1.2 Exposure to noncarcinogens in groundwater

The COVs for ingestion, inhalation, and dermal contact pathways for groundwater are 0.58, 0.4 and 0.26, respectively. These values are less than 1; therefore, the expected variation in the model predictions are not expected to be very wide. The predicted maximum risks vary, at most, by one order of magnitude from the predicted minimas because the impact of the most varying parameter (i.e., the exposure duration) in the carcinogenic model is screened out by an equivalent variation in the averaging time. This is the case for shorter term exposures where the impact of the averaged exposure over the life time of the receptor is not a significant factor. Therefore, models used to predict risk from exposure to noncarcinogens are not widely varying with variations of the uncertain parameters.

For the ingestion pathway, sensitivity analysis shows that the sensitivity in the risk prediction is 83% from the uncertainty in the water ingestion rate. The body weight and the exposure frequency have a limited impact (10 and 6%, respectively) on the predicted risk.

For the inhalation pathway, sensitivity analysis shows that the variation in the risk prediction is 74% from the uncertainty in the inhalation rate. The body weight and the exposure frequency have a limited impact (14

and 12%, respectively) on the predicted risk.

Sensitivity analysis for the dermal contact pathway shows that variation in the risk prediction is 53% due to variations in the exposure time, 31% due variation in the exposure frequency, and 15% due to variation in the surface area to the body weight ratio.

H.4.1.3 Exposure to radionuclides in groundwater

The COVs for ingestion of contaminated groundwater is 1.33. This value reflects a variation of three orders of magnitude between the maximum and minimum predicted risk results (see Table H.4). Sensitivity analysis shows that the variation in the risk prediction is 79% from the uncertainty in the exposure duration parameter, 18% from the ingestion rate of water, and a negligible contribution from the exposure frequency (2%).

H.4.2 Soil Pathways

Table H.6 presents a descriptive statistical analysis of the Monte Carlo simulations of the risk predictions associated with the uncertainties in the input parameters for the soil exposure models. The point estimate of the risk calculations and the ratios between the point estimates and the 95th and 97.5th percentiles are given.

Table H.6. Results of the uncertainty analysis for the soil exposure pathways

	Carcinogens			Noncarcinogens				Radionuclides	
Statistics	Ingestion	Inhalation	Dermal	Ingestion-ad	Ingestion-ch	Inhalation	Dermal	Ingestion	External
COV	1.01	1.24	2.95	0.65	0.88	0.44	1.65	0.84	1.24
Minimum	3.1 E-9	6.2E-7	3.5 E-10	8.2E-10	1.1E-7	3.2E-5	9.3 E-9	2.2E+0	2.3E-2
50%	1.2E-7	1.2E-5	5.5E-8	7.0E-8	2.3E-6	1.2E-4	5.1E-7	6.3E+1	3.4E+0
95%	4.7E-7	6.5E-5	6.4E-7	1.9E-7	8.3E-6	2.2E-4	3.6E-6	2.1E+2	1.8E+1
97.5%	5.8E-7	8.7E-5	1.3E-6	2.2E-7	1.0E-5	2.3E-4	5.3E-6	2.6E+2	2.5E+1
Maximum	2.0 E-6	2.7E-4	1.3 E-5	3.4E-7	2.7E-5	3.3E-4	2.4E-5	5.8E+2	7.3E+1
Point Estimate	1.6E-6	1.2E-4	1.1E-6	1.4E-6	1.3E-5	2.7E-4	2.7E-6	1.3E+3	2.3E+1
PE/(95%)	3.3	1.8	1.8	7.2	1.6	1.3	0.7	6.0	1.3
PE/(97.5%)	2.7	1.34	0.9	6.4	1.3	1.2	0.5	4.8	0.9

This table shows that for both nonradioactive and radioactive carcinogens the COVs are greater than one, which implies multiple orders of magnitude of variation over the range of the model predictions. For noncarcinogens, the variability in the model predictions was much less.

The relative risk ratio is calculated to determine the location of the point estimates with respect to the uncertainty predictions of the individual models. The calculations of relative risk ratios, the ratio of the PE to the predicted percentiles, show that the PEs lie in the last 2.5% predictions of the Monte Carlo simulations for different exposure pathways. In the following subsections, the individual pathway ratios are evaluated, and the PE/MEF ratios are assessed.

Table H.7 presents the corresponding sensitivity analysis of the risk predictions associated with uncertainties in the input parameters for all soil models presented in Sect, 2. Note that sensitivity results exceeding 1% contribution only are presented in Table H.7.

Table H.7. Results of the sensitivity analysis for the soil exposure pathways

	Carcinogens			Noncarcinogens				Radionuclides	
Sensitivity data	Ingestion	Inhalation	Dermal	Ingestion-ad	Ingestion-ch	Inhalation	Dermal	Ingestion	External
FI_{ch}	**31%**	.	.	.	**43%**	.	.	**24%**	.
ED_{ch}	**29%**	.	.	.	.	.	.	**24%**	.
IR_{ch}	**29%**	.	.	.	**45%**	.	.	**25%**	.
BW_{ch}	6%	.	.		8%	.	.	.	.
EF	3%	2%	1%	6%	3%	**12%**	2%	5%	2%
IR_{ad}	1%	1 %	.	**47%**	.	.	.	5%	1%
ED_{ad}	1%	**84%**	**36%**	.	.	.	.	**15%**	**82%**
FI_{ad}	.	.	.	**42%.**	.	.	.	3%	.
SABW	.	.	1%	6%	.		2%	.	.
BW	.	2%	.	.	.	**14%**	.	.	.
Se	.	.	.	.	.	.	.	.	**15%**
IR_{air}	.	**11%**	.	.	.	**74%**	.	.	.
AF	.	.	**61%**	.	.	.	**96%**	.	.

This table shows that several parameters are found to be significant for each pathway. Therefore, to reduce the range of variation in each model, and therefore to increase the confidence in the predicted risk values, the statistical information of the most sensitive parameter in the model of concern must be considered. The sensitivities exceeding 10 % contributions are bolded. The following subsections elaborate on the risk results for each pathway for the carcinogenic, noncarcinogenic, and radioactive exposure models.

H.4.2.1 Exposure to nonradioactive carcinogens in soil

The COVs for ingestion, inhalation, and dermal contact pathways for groundwater are 1.01, 1.24 and 2.95, respectively. Since these values deviate from zero, the expected variation in the model predictions are expected to be wide. For the ingestion and inhalation pathways, the predicted maximum risks vary by two to three orders of magnitude from the predicted minimas. The dermal contact pathway range of variation is even wider (almost five orders of magnitude) and the confidence in the distributions of the most sensitive parameters in this model have to be examined in greater detail to see whether they can be more fined based on additional data.

For the ingestion pathway, sensitivity analysis shows that the most sensitive parameters are fraction ingested, exposure duration, and ingestion rate of a child with contributions of 31, 29, and 29 %, respectively, to the exposure model. The exposure prediction sensitivity associated with variations in the exposure

parameters that pertains to the adult exposure scenario are insignificant.

For the inhalation pathway, sensitivity analysis shows that the exposure duration is the most sensitive parameter with an 84% contribution to the sensitivity of the predicted risk. Additionally, the distribution of the inhalation rate has a limited impact (11%) on the sensitivity of the predicted risk.

Sensitivity analysis for the dermal contact pathway shows that the variation in the risk prediction is 61% governed by the lognormal distribution of the adherence of soil-to-skin factor. The next important parameter is the exposure duration with a sensitivity of 36%.

The PE/MEF ratio, the ratio of the point estimate to the predicted percentiles of the multiplicative exposure factor, show that the PE for the ingestion risk is 2.7 of the 97.5% predictions of the Monte Carlo simulations. In fact, the PE lies closer to the 99% prediction for the ingestion pathway. Additionally, the point estimates for the inhalation and the dermal contact risks lie in the 2.5% predictions (i.e., 1.34, and 0.9 of the 97.5% predictions, respectively) of the Monte Carlo simulations.

H.4.2.2 Exposure to noncarcinogens in soil

The COVs for adult ingestion, child ingestion, inhalation, and dermal contact pathways for groundwater are 0.65, 0.88. 0.44, and 1.65, respectively. For the ingestion pathways, the predicted maximum risks vary by two orders of magnitude from the predicted minimas; for the inhalation pathway, the variation is by one order of magnitude; and for the dermal contact pathway, the range of variation is more than four orders of magnitude. Note that the COVs are again reduced to less than 1 because the impact of the most varying parameter (the exposure duration) is screened out by an equivalent variation in the averaging time. Therefore, models used to predict risk from exposure to noncarcinogens do not show as much variation as exposure models used to calculate carcinogenic risk estimates.

For the adult ingestion pathway, sensitivity analysis shows that the most sensitive parameters are the ingestion rate and the fraction ingested with contributions of 47 and 42%, respectively, to the risk model. For the child ingestion pathway, the sensitivity of the predicted risk to the ingestion rate and the fraction ingested is 43 and 45%, respectively. The risk prediction sensitivity associated with variations in the other exposure parameters is negligible.

For the inhalation pathway, sensitivity analysis shows that the variation in the risk prediction is 74% from the uncertainty in the water inhalation rate. Body weight and the exposure frequency have a very limited impact (14 and 12%, respectively) on the predicted risk.

Sensitivity analysis for the dermal contact pathway shows that variation in the risk prediction is mainly associated with variations in the adherence of soil-on-skin factor (96%).

The calculations of the PE/MEF ratio show that the PE for the adult ingestion risk is 6.4 of the 97.5% predictions of the Monte Carlo simulations. The PE is actually observed to be considerably outside the range of the Monte Carlo prediction (by more than four times). For the child ingestion pathway, the PE almost lies at the 97.5% prediction (relative risk ratio of 1.3). Additionally, the point estimate for the inhalation pathway lies in the last 2.5% predictions (i.e., 1.2 of the 97.5% predictions) of the Monte Carlo simulations. For the dermal pathway, the relative risk ratio 0.7 at 95% tile. Therefore, PE is expected to lie closer to the 92.5% tile of the Monte Carlo simulation.

H.4.2.3 Exposure to radionuclides in soil

The COVs for ingestion of and external exposure to contaminated soil with radionuclides are 0.84 and 1.24. This value reflects a variation of two to three orders of magnitude between the maximum and minimum predicted risk results (see Table H.5).

Sensitivity analysis shows that the variation in the risk prediction from the ingestion of contaminated soil with radionuclides is attributed to variations in several exposure parameters. Equal contributions of 25% were from the ingestion rate, exposure duration, and ingested fraction that pertains to the child exposure scenario; 15% came from variations in the exposure duration of an adult.

For the external exposure pathway, the predicted risk is most sensitive to variations in the adult exposure duration (82%). The shielding factor contribution to the sensitivity of predicted risk is 15%.

The calculations of relative risk ratio show that the PE for the ingestion risk is almost 5 times the 97.5% predictions of the Monte Carlo simulations. Actually, the PE is observed to be outside the maximum range of the Monte Carlo prediction by more than two times. For the external exposure pathway, the relative risk ratio is 0.9 at the 97.5% tile.

H.5. RISK MANAGEMENT APPLICATION

It is widely recognized that the values used to generate point risk assessment results are conservatively biased (e.g., Burmaster and Harris 1993) and often yield an exposure estimate that is greater than the 99th percentile. Indeed, the results documented here show that point estimates can be as high as 4 times the maximum of the range of the Monte Carlo analysis for some pathways. However, the attempts at Monte Carlo analyses for sites are often confounded by site-specific and contaminant-specific factors related to estimates of the concentration term and in difficulties in estimating the dose-response relationship. Therefore, Monte Carlo analyses are not often implemented for particular sites. By segregating the uncertainties that are specific for the exposure parameters in a particular land use scenario from those that are site- and contaminant-specific, the assessor can work to reduce the uncertainties associated with the site while being able to recognize the uncertainties inherent in the exposure process.

A 90–95th percentile value of the forecast distribution can be used to determine a multiplicative exposure factor that is specific for each pathway of each land use scenario. If these values were developed for all pathways of each land use scenario, the risk assessment process itself could be greatly simplified. For example, the risk for the ingestion pathway could be expressed as the product of the exposure concentration, a dose-response relationship, and the multiplicative exposure factor rather than using all of the parameters presented in Sect. H.2. This would translate to direct cost savings through easier generation of risk estimates and by reducing the amount of quality assurance that is currently necessary to ensure that the risk estimates are free of error. In addition, use of percentiles of the multiplicative exposure factors would maintain the advantages of the point estimate approach in terms of their interpretability by the general public while being more indicative of an estimate that is protective of 90–95% of the potentially exposed population. Of course, it is not necessary to employ Monte Carlo analyses to produce MEFs based on current EPA guidance. Table H.5 gives values for the EPA default point estimates that can be used as MEFs. However, Table H.5 also shows the extent of conservatism that is built into many of the pathways. Use of the default factors can cost significant amounts of money in essentially cleaning up to criteria that far surpass the risk management goals.

While this methodology could be applied at the vast majority of sites, it is recognized that there are sites where local exposure patterns deviate significantly from national norms. For these sites (e.g. fish consumption among Native Americans), this method would not be applicable and the distributions and resulting percentiles would have to be modified to reflect local exposure patterns. However, the vast majority of sites fall under the same general EPA guidance recommendations for exposure patterns and use of this method would result in more reliable risk estimates at less cost.

H.6. CONCLUSIONS

Uncertainties in the risk predictions from exposure to contaminated groundwater and soil have been evaluated for the residential scenario in this report. The variability and the sensitivity of the EPA Superfund exposure model predictions to the input parameters has been examined and documented. In addition, the confidence and conservatism of the point estimates with respect to the probabilistic estimates have been evaluated by calculating a relative risk ratio between the PE and the closest percentile prediction of the multiplicative exposure factor.

H.6.1 Groundwater Models

For the ingestion, inhalation, and dermal contact exposure pathways to nonradioactive carcinogens and for the ingestion of radioactive carcinogens in groundwater the COVs tend to be greater than 1, which reflects orders of magnitude of variation between the minimum and the maximum predictions of the multiplicative exposure factor. The corresponding results of the sensitivity analysis show that the exposure duration is the most sensitive parameter and is the main cause of the wide variability of the predictions. Current studies on an acceptable distribution for the exposure distribution supports the distributions used in this study; therefore, the large standard deviations are an acceptable representation of the parameter variation and the expected variation is the model predictions are justifiable. However, point estimate to multiplicative exposure factor ratios at the 97.5% tiles for these pathways imply that the PEs are highly conservative.

For the ingestion, inhalation, and dermal contact exposure pathways to noncarcinogens in groundwater, the COVs tend to be less than 1, which reflects a smaller range of variation between the minimum and the maximum predictions of the exposure model. The corresponding results of the sensitivity analysis show that the ingestion rate and the inhalation rate are the main parameters of concern for the ingestion and inhalation pathways. The exposure time and exposure frequency are the most sensitive parameters for the dermal pathway model. The relative ratios for the point estimates and the 97.5th percentiles for these pathways imply that the EPA default point estimates are conservative and generally result in an overestimate of the actual risk.

H.6.2 Soil Models

For the ingestion, inhalation, and dermal contact exposure pathways to nonradioactive carcinogens in soil, the COVs tend to be greater than 1, which reflects the orders of magnitude of variation between the minimum and the maximum predictions of the model. The corresponding results of the sensitivity analysis show that several parameters are contributing to this wide range of variation (refer to Table H.7). The relative risk ratios lie closer to the 99% tile for the ingestion pathway and 97.5% tiles for the inhalation and dermal contact pathways. This implies that the point estimates for the exposure parameters recommended by EPA are highly conservative.

For the adult ingestion, child ingestion, and dermal contact exposure pathways for noncarcinogens in soil,

the COVs reflect a wide range of variation between the minimum and the maximum predictions of the model. The smallest variation is observed in the inhalation pathway. The corresponding results of the sensitivity analysis show that the ingestion rate and the ingested fraction and the inhalation rate are the main parameters of concern for the ingestion and inhalation pathways, respectively. The adherence of soil-on-skin factor is the most sensitive parameter for the dermal contact pathway model. The relative ratio of the point estimates to the Monte Carlo percentiles for the adult ingestion pathway show that the point estimate occurs outside the wide range of predictions. This implies that the point estimates provided by EPA for this pathway are extremely conservative. The relative risk ratios at the 97.5% tiles for the child ingestion and inhalation pathways imply that the PEs are still conservative. For the dermal contact pathway the point estimate is expected to lie closer to the 92.5% tile of the Monte Carlo simulation.

For the ingestion and external exposure pathways to radioactive carcinogens in soil, the COVs reflect orders of magnitude of variation between the minimum and the maximum predictions of the model. The corresponding results of the sensitivity analysis show that several parameters are contributing to this wide range of variation (refer to Table H.7). The relative risk ratio for the ingestion pathway show that the point estimates are greater than the maximum of the predictions. The relative risk ratios lie closer to the 97.5% tile for the external exposure pathway. This again implies that the EPA point estimates are highly conservative.

An alternative to the continued use of conservative point estimates is the use of a 90–95th percentile value of the forecast distribution of the multiplicative exposure factor. These can be developed specifically for each pathway of each land use scenario. These values could greatly simplify the risk assessment process through easier generation of risk estimates and by reducing the amount of quality assurance that is currently necessary to ensure that the risk estimates are free of error. These two factors would decrease the dollar amount that a risk assessment costs to produce. Reducing the inherent conservatism in the risk estimates would also translate to reduced costs in implementing remedial action alternatives while still meeting stated risk management goals through the Superfund decision process. In addition, use of percentiles of the multiplicative exposure factors would maintain the advantages of the point estimate approach in terms of their interpretability by the general public while being more indicative of an estimate that is protective of 90–95% of the potentially exposed population.

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APPENDIX I

INTEGRATION POINT ASSESSMENT METHOD

The first step in performing the integration point assessment is selecting the actual point of assessment. In general, an integration point assessment should be performed for systems that drain catchment areas at the boundaries of the ORR. Examples include White Oak Lake, East Fork Poplar Creek, Bear Creek, Poplar Creek, and the Clinch River. These large-scale integration point assessments can assist in prioritizing activities at known contaminant sources. Other points can be selected as needed to support activities taken to control contaminant sources. Integration point assessments can be used to support remedial investigations and may assess only a portion of the larger integrator watershed to ensure that remedies for smaller subsystems of the watershed achieve acceptable risk levels.

The integration point assessment is then performed at the chosen point using the 95% upper confidence limit on the arithmetic average for yearly concentration data. Surface water pathways are assessed at this point with the assumption of residential land use of the water. This would entail using standard risk assessment parameters that are available in *Risk Assessment Guidance for Superfund, Part A: Human Health Evaluation Manual* (EPA 1989) for these pathways.

Primary pathways to be assessed include ingestion of surface water, dermal contact while showering, and indoor inhalation of chemicals resulting from water use. The cumulative risk across all pathways for all chemicals at this point is then compared with an excess lifetime cancer risk (ELCR) of 1E-04 and to the noncarcinogenic hazard index of 1 to determine the need for early action. If these risk and hazard levels are exceeded, potential early actions may be evaluated. Also, contaminant fluxes and risk are used to identify the primary contributors to the risk at the integration point and prioritize the contributors to the risk.

Generally, the results generated by a risk assessment are driven by a few high priority chemicals. Determination of high priority chemicals can be achieved by selecting those chemicals or elements comprising 90% of the total risk at the integration point. For chemicals that drive the risk, the annual fluxes for each should be quantified to the degree possible at the integration point and at the major source areas. The spatial resolution of the source areas is dependent upon the amount of source data available.

The flux data for each of the source areas are then used with the integration point flux data to rank the relative importance of the different source areas within the context of the integration point. Given the generalized cancer risk equation for multiple substances:

$$Risk_T = \sum Risk_i ,$$

where:

$Risk_T$ = the total cancer risk, expressed as a unitless probability,
$Risk_i$ = the risk estimate for the i^{th} substance.

The equation for calculation of carcinogenic effects for the flux-based risk assessment at each of the sources is:

$$Risk_{sf}\ (\%) = \{\sum [\ Risk_i\ (Flux_{is} / Flux_{ip})]\} / Risk_T ,$$

where:

$Risk_{sf}$ = percentage of risk at the integration point that originates at the source,
$Flux_{is}$ = flux of the i^{th} substance originating at the source,

$Flux_{ip}$ = flux of the i^{th} substance identified at the integration point.

Similarly, the standard equation for calculation of noncarcinogenic effects is:

$$\text{Hazard Index}_t = \sum E_i/RfD_i$$

where:

E_i = exposure level (or intake) for the i^{th} toxicant,
RfD_i = reference dose for the i^{th} toxicant;

where: E and RfD are expressed in the same units and represent the same exposure period (i.e., chronic, subchronic, or shorter term).

The calculation for the flux-based risk assessment of noncarcinogenic effects is:

$$\text{Hazard}_{sf}\ (\%) = \sum[\ E_i Flux_{is}/RfD_i Flux_{ip}]/\text{Hazard Index}_t\ ,$$

where:

$Hazard_{sf}$ = percentage of the hazard index at the integration point that originates at the identified source.

Although carcinogenic and noncarcinogenic results from the integration point assessment are typically presented in the same format (i.e., as a % of the $\sum$), it should be noted that carcinogenic and noncarcinogenic effects cannot be combined if the integration point assessment indicates that both are of concern. This is due to the difference in health effects associated with carcinogens and noncarcinogens.